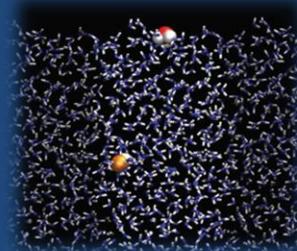
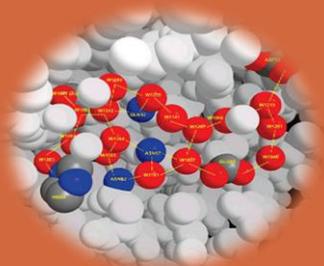
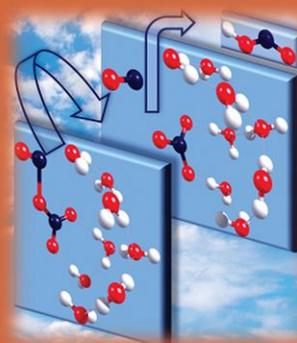


The Hebrew University of Jerusalem
The Fritz Haber Research Center for
Molecular Dynamics



Annual Report

2009



PRESENTED TO THE SCIENTIFIC ADVISORY COMMITTEE, THE BEIRAT

G. Meijer (Chair)
S. Arkin
M. Asscher
E. K. U. Gross
H. Grubmüller
N. Moiseyev
A. Nitzan

July 2010

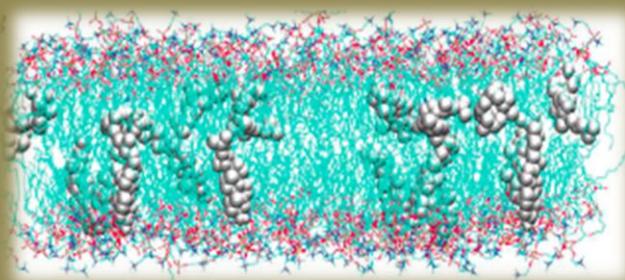


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INTRODUCTION

The Fritz Haber Research Center is the first Minerva center inaugurated at the Hebrew University of Jerusalem. The center is an assemblage of ten scientific research groups, each headed by a university faculty member. The total number of researchers, including MSc. PhD. students and postdocs is about 50.

The key activity of the Fritz Haber center is theoretical and computational research of chemical systems, with particular emphasis on dynamics and molecular processes. The various research endeavors span a broad variety of topics impacting diverse fields such as biology, environmental sciences, materials science and laser physics.

The Fritz Haber center is a basis of operations for a variety of bustling research activities. It furnishes the researchers at the center with basic services which the university has almost ceased to provide. The center bestows a scientific ambience which is in many ways unique in the institute of chemistry or perhaps the entire university. The center holds a bi-weekly seminar, hosting world-leading scientists as well as young researchers and graduate students. The center has also organized and sponsored numerous scientific symposia and conferences (a detailed list of recent years' activity appears in Part III). Each year several short-term visitors and long-term collaborators come for brief visits from other universities in Israel and abroad. Over the years, more than a hundred graduate students completed their doctoral theses in the center, and a comparable number of post-graduate students from many countries began here their training as independent researchers. Many of our former students and postdocs now hold academic positions at first rate academic institutions in various countries, including Israeli universities such as the Weizmann Institute, the Technion, Tel Aviv University and the Hebrew University. Others occupy leading positions in industrial and governmental institutions.

Over the years the center has been cultivating a vibrant collaboration with many science groups in Germany. Furthermore, many of our visitors are from Germany, among them Minerva fellows who are now faculty members at various German academic institutes. The students, postdocs and our more senior collaborators in Germany and other countries have contributed to the numerous research articles (more than 1400), reviews, and books published by the members of the center, many of which have been frequently cited and used by other researchers around the world. It should be stressed that the affiliation 'Fritz Haber Center' appears as part of the authors' address in all of these publications. Lists of publications during the last five years, as well as a list of visitors and seminars are given in Part III of this report.

The principal research tool used by the scientists at the center is the computer. The computing unit of the center includes a large number of clusters composed of hundreds of computer nodes of varying strengths and capabilities. The smooth operation of the computers and is overseen by one system manager, with a part time "soft money" assistant. More on the services and capabilities of our computer facility is given in Part II of this report.

The administrative activities in the center are coordinated by one staff member with occasional part time help. Additional details about the history of the center, personnel, budget, etc. are given in Part II of this report.

HISTORY OF THE CENTER

The Fritz Haber Research Center for Molecular Dynamics was established by the Minerva Society and The Hebrew University to strengthen the synergy between theory and experiment, to support research in molecular dynamics and to encourage cooperation between German and Israeli scientists. The center, which supports

theoretical research in most branches of chemical and molecular physics, began its activities in January 1981. The agreement between The Minerva Society of the Federal Republic of Germany and the Hebrew University, providing an endowment fund for the Fritz Haber Research Center, was signed in August 1981. The computer facility started operation in November 1981. The official inauguration of the Center took place on May 26, 1983. The initial endowment fund was 1,000,000 DM. On the occasions of the fifth anniversary of the Center in 1986 and the tenth anniversary in 1991, Minerva announced increases in the endowment fund. In 1986 the endowment was increased by 1,000,000 DM and in January 1992 by an additional sum of 500,000 DM. In July 1997 the endowment was increased again by 1,000,000 DM. The annual budget of the center stems from the endowment's interest, matched by Hebrew University support. Because of the drastic drop in interest rates and the decrease in USD/EU exchange rate, the average annual budget which was about 200,000 EU until 2001, has dropped to about 75,000 EU in recent years.

It should be emphasized that the entire budget is dedicated to the joint activities of the center and its infrastructure. In addition, members of the center are funded by external agencies on a per-project basis. There are about 30 such current projects, with a total annual budget of over 800,000 USD.

At inception, headed by its first director, Professor Raphael D. Levine, the Fritz Haber center numbered ten members and a similar number of associate members, including both experimentalists and theoreticians from the Hebrew University and other universities in Israel. Professor Dr. Edward W. Schlag has served as the first Chairman of the center's scientific advisory board (the Beirat) and accompanied its activities and development until 1998, and contributed substantially to its recognition as a leading center of theoretical chemical physics. During 1989-1991 the Director of the center was Professor Robert B. Gerber and he was followed by Profes-

or Ronnie Kosloff (1991-1998). In 1998 Professor Avinoam Ben-Shaul was appointed the Director and in parallel a new Beirat was formed chaired by Professor Dr. George Comsa. Under his leadership this new Beirat continued to support, guide and nourish the center's development. We would also like to acknowledge the contributions of Professors Erich Sackmann, Jurgen Troe, Hanoch Gutfreund and Joshua Jortner who served as Beirat members for many years, and devoted their time and shared their experience to encourage the scientific activity of the center. Professor Dr. Wolfgang Domcke was the Chairman of the Beirat in the years 2005-2009. In 2010 the Professor Dr. Gerard Meijer was appointed chair of the Beirat.

In 2006 Dr. Daniel Harries joined the center following his appointment as a senior lecturer. In 2007 Professor Roi Baer joined the center as its Director. In 2009 Dr. Masha Niv and Dr. Assaf Zemel, both former students of the center and now freshly appointed senior lecturers joined the center. These new recruits have broadened and updated the domain of operations at the center, with new fields of research, such as cell dynamics, protein dynamics, molecular electronics and electronics structure of semiconducting nanocrystals and metal nanoparticles.

Sadly, in 2009, Professor Victoria Buch died of cancer at the age of 55. The center helped organize a symposium, as her scientific collaborators and friends from around the world gathered to commemorate Professor Buch and her scientific contributions.

THE BEIRAT

The Beirat oversees the operations of the Center and offers guidance to its director. Annually, the center submits a report to the Beirat, detailing the scientific progress and activity, as well as a financial report and a budget proposal for the next year. The Beirat is requested to report to Minerva on the program, budget and activities of the Center.

The Beirat convenes every second year. The last meeting was held in Jerusalem in June 2009 and included a successful international symposium on Biophysical Dynamics.

The Members of the Beirat are:

- Professor Dr. G. Meijer (Berlin, Germany), Chairman
- Professor Dr. E. K. U. Gross (Halle, Germany)
- Professor Dr. H. Grubmüller (Göttingen, Germany)

- Professor S. Arkin, (Jerusalem, Israel, Vice President for R&D, Hebrew University).
- Professor M. Asscher (Jerusalem, Israel)
- Professor N. Moiseyev (Haifa, Israel)
- Professor A. Nitzan (Tel-Aviv, Israel)

The members of the center would like to thank present and past members of the Beirat for their constant advice, encouragement, constructive criticism and support through all the years, some of which were difficult in many respects.

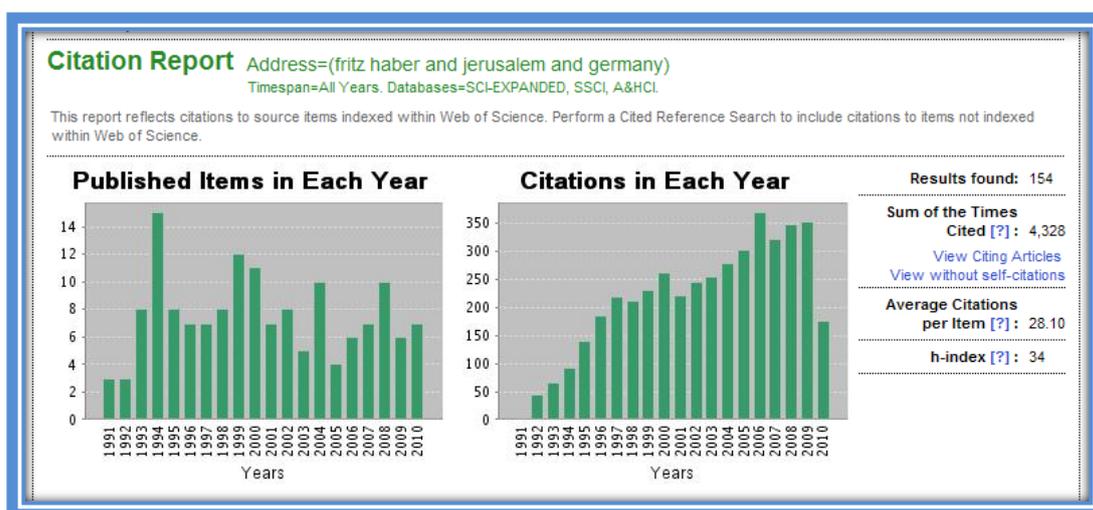
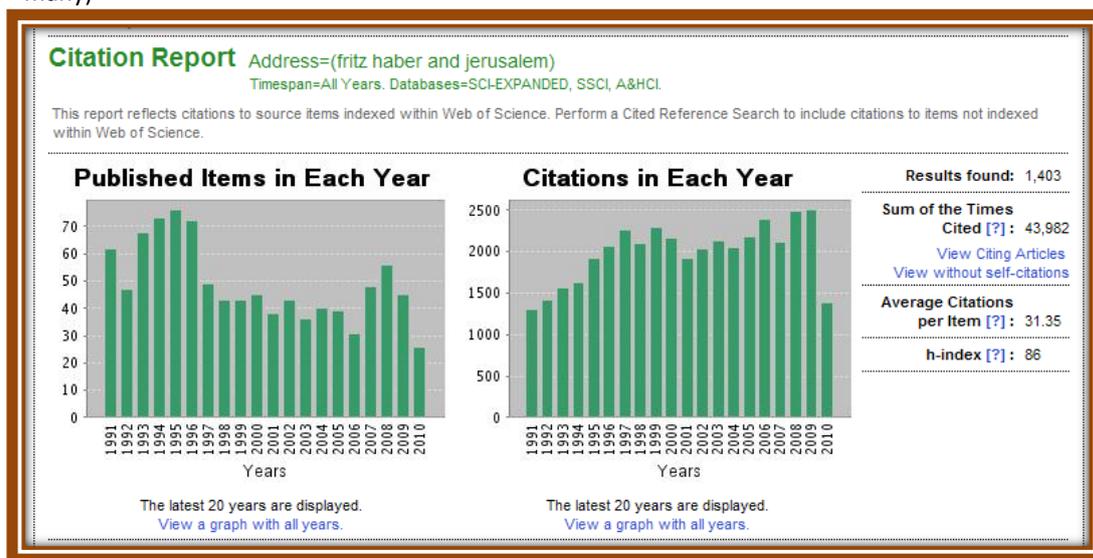


Figure 1: Top: Citation report for the Fritz Haber Center (latest 20 years). Bottom: Citation report for joint Fritz Haber center and German publications.

STATISTICS OF SCIENTIFIC IMPACT

Since its inauguration the researchers of the center have published over 1400 scientific articles in

refereed journals with direct affiliation to the Fritz Haber Minerva Research Center. These articles were cited in the scientific literature 44,000 times with an average of 31 citations per

paper and an h-index of 86 (see Figure 1). The citation rate is 2500 per year and about 50 papers are published each year. The collaboration with German scientist is intense, culminating in over 150 papers which were cited over 4300 times with an average of 28 citations per item.

PAST EVALUATION COMMITTEES

The scientific activities of the center have been extensively reviewed, twice, by international evaluation committees composed of world leading scientists. The first Minerva review was held in 1994 by a committee headed by Professor H. Schwarz and the second in 2002 headed by Professor Dr. H. –J. Werner. The members of the second evaluation committee were Professors E. J. Heller, W. H. Miller, M. Parrinello and K. Schulten. In both reviews, the reports have been extremely enthusiastic, praising the achievements of the center. The reviews also provided useful advice about possible ways to improve the center's activities. Both committees have also recommended an increase of the Center's endowment as well as granting a special equipment fund. In 1994 this has indeed lead to a substantial increase of the budget and upgrading of equipment. Owing to budgetary cuts the recommendations of the second committee could not be met. In this regard we should mention that the annual operation budget of the Fritz Haber center in recent years is ca. \$130,000, which constitutes a relatively small fraction (about 15%) of the total operation budget of the groups in the center. While modest, this budget is essential, since this is the only source of sup-

port for our *joint activities*, such as the exchange of students and visitors with Germany (several of our German collaborators are affiliated with several groups of the center), maintenance of computing equipment, seminars and symposia, as well as the salaries of our administrator and that of the system-managers. At the end of year 2006 the Minerva Evaluation Committee met with the Hebrew University centers. The committee visited the Fritz Haber center, met with its members and a detailed overview of the activities and future plans of the center was presented.

In 2009 Minerva requested the center to submit a septennial report (2002-2008) and the Beirat, then headed by Prof. Dr. W. Domcke, to submit an enlarged report. In the report, the Beirat summarizes as follows:

"In the opinion of the Beirat, the Fritz Haber Research Center is still going very strong 29 years after its inauguration. All of the members perform cutting-edge research in up-to-date areas and several of them are international stars. The Fritz Haber Center is a true center of excellence. It is very sad that Victoria Buch passed away recently at the peak of her scientific performance after a long struggle with a fatal disease.

In summary, the Beirat strongly endorses the continuation of the funding of the Fritz Haber Research Center at the Hebrew University. In addition to an increase of the declining budget, funds should be made available for the modernization and sustenance of the computational facilities of the center."

PART I: ANNUAL SCIENCE REPORT, 2009

Originally, and in accordance with its name, research at the center has been mostly concerned with molecular reaction dynamics and closely related topics, such as laser-molecule and surface-molecule interactions. In the spirit of the period, the research has focused on processes involving small molecules and state-to-state processes, usually in the gas phase. Twenty five

years later, part of the research carried out at the center is still concerned with molecular rate processes but emphasis has shifted towards larger and more complex systems.

Today, the characterizing theme of the center is its extremely diverse fields of operations, encompassing practically all aspects of molecular

dynamics. Temperature-wise, our research starts from 10^{-9} °K, with chemical reactions of Bose-Einstein condensates; through the **1-100°K** regimes with noble-gas molecules and molecular electronic devices operate; below the water freezing point **0 °C** regime for ice surfaces, and warming up to room temperature regimes where biological diversity rules; things then really start to cook up at around 1000°K which are characteristic of the diamond formation environment within Earth's Mantle; and finally intense heating up to 10^5 °K, the effective temperatures achieved by powerful short pulse lasers which cause Coulomb explosion of molecules. Some of the research topics covered by the center are:

- Chemistry at water and ice surfaces
- Proton transfer processes
- Complex fluids
- Protein structure and dynamics
- Assembly mechanism of viral particles
- Cell locomotion
- Molecular electronics
- Optical properties of nano-crystals
- Light-matter interactions and plasmonics
- Optimal Coherent Control
- Chemistry of Bose Einstein condensates
- Attosecond electron dynamics

This enlargement of scientific goals for the center has been approved, even encouraged, by past evaluation committees, in 1994, 2002 and the extended 2002-2008 Beirat report. Indeed, we find that while strong expertise and the existence of a 'critical mass' of researchers in a specific field (molecular dynamics in our case) is imperative for success, the dialogue with researchers in neighboring fields of science is invaluable. Similarly, as attested by many joint publications, close collaboration with experimental groups is a characteristic of all research groups at the center.

The phenomena of interest, dealing mainly with dynamical, kinetic, and radiative processes, also involve a wide spectrum of inter-particle interactions and diverse molecular properties. A number of research projects are concerned with quantum effects such as chemical selectivity mediated by the coherent control of laser-matter interaction, ultra cold (nano K) chemistry, or novel architectures of quantum dots towards the development of chemically synthesized computers. At least four groups at the Center are engaged in the research of molecular or metallic clusters. These studies include the dynamics and thermodynamics of cluster-surface encounters and, on a more microscopic level, the internal dynamics, structure, spectroscopy and photochemistry of molecular clusters, especially water oligomers and ion-water complexes.

The theoretical understanding of the systems and phenomena mentioned above requires the development of new theoretical methods and sophisticated computational algorithms. Thus, all members of the Center are continuously involved in such developments and our recruitment efforts put strong emphasis on this aspect. Their record of theoretical contributions to molecular reaction dynamics, quantum nuclear dynamics, quantum electron dynamics, algebraic methods, coherent control, statistical and information theoretic approaches, diffusion kinetics, spectroscopy, quantum chemistry, protein structure and dynamics, as well as the statistical thermodynamics of complex fluids and biophysical systems are all well recognized internationally.

In the remainder of this chapter we provide a detailed scientific report concerning the research done in each of the groups of the center. The topics studied are also reflected in the lists of publications given in Part III.

INDIVIDUAL RESEARCH PROGRESS REPORTS

NOAM AGMON

Our main research theme in 2009 involved proton migration along hydrogen bonds (HBs) termed "proton wires", both in liquid water and in proteins.

SCIENTIFIC PROJECTS

WATER WIRES CONNECTING ACID-BASE PAIR

In a collaborative work with the experimental group of Huib Bakker from Amsterdam we have analyzed proton transfer (PT) kinetics (measured by time resolved IR) between a photo-acid (HPTS) and relatively high concentrations of a moderate base (acetate) in liquid water. Under these conditions, the acid-base pair comes into close proximity before the proton has time to transfer to solution, so that the kinetics is governed by direct PT between acid and base rather than by proton transfer to solvent. Since this transfer is irreversible, it falls into the realm of pseudo-unimolecular reactions traditionally treated by the Smoluchowski theory. However, it was found in earlier experiments, both in the Nibbering and Bakker groups, that the Smoluchowski model with contact reactivity cannot fit the observed kinetics (dashed lines in Figure 2). This was attributed to PT via water-wires connecting the proton acceptor and donor at close proximity. However, the kinetic models utilized were rather involved and could not fit the data over the whole observation time in a consistent manner. In particular, one observes in Fig. 1 that the signal from the photoacid decays abruptly on the fs timescale and then much more gradually on the 100 ps timescale.

It is apparent that the short behavior could be attributed to PT between static acceptor and donor pairs with distance dependent reactivity, whereas at longer times the reaction is limited by the diffusion of such pairs which need to come into closer proximity. This can be addressed by a modified Smoluchowski model in which the delta-function sink term is replaced by a dis-

tance-dependent one. This makes PT resemble electron transfer reactions more closely. However, we find that a Gaussian sink term allows us to obtain better fits to the fs kinetics, and this differs somewhat from the exponential sink traditionally utilized in electron transfer. Since the model has a built-in diffusion term, it switches over to diffusion influenced kinetics in the ps timescale, so that one model explains the data on all timescales, as seen by the full lines in Figure 2.

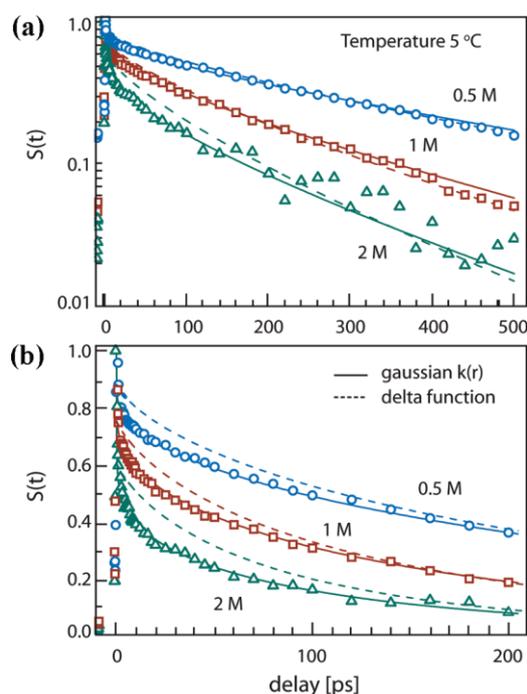


Figure 2: Survival probability of excited hydroxypyrene-trisulfonate (HPTS) in aqueous solutions of various concentrations of acetate at room temperature.

We have also investigated the temperature dependence of this reaction, which was not done in the previous time-resolved IR experiments. Interestingly, we find that the Gaussian sink terms slow-down with increasing temperature, rather

than speeding-up as expected from Arrhenius kinetics (Figure 3). This suggests that the transfer is a coherent quantal process rather than a sequential hopping process as suggested by earlier studies. We propose that the proton moves concertedly over water wires composed of several water molecules. As the temperature is raised, the HBs along these wires tend to break more often, thus impeding the through-wire PT process.

- ❖ M. J. Cox, R. L. A. Timmer, H. J. Bakker, S. Park and N. Agmon, *J. Phys. Chem. A* 113, 6599–6606 (2009).

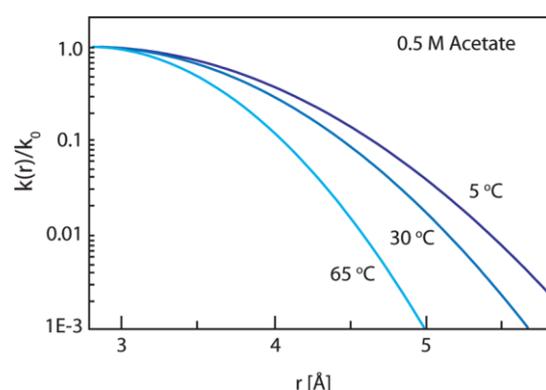


Figure 3: Distance dependent rate-coefficient for PT between excited HPTs and 0.5 M acetate at different temperatures. The Gaussian $k(r)$ is depicted here on a semi-log scale. Note how, except at contact, $k(r)$ diminishes with increasing T .

PROTON WIRES IN CARBONIC ANHYDRASE AND GFP

A program for mapping proton wires in proteins has been developed by Mrs. Ai Shinobu during her M.Sc. work. Protons cannot migrate, like electrons, in vacuum or along the sigma bonds of a protein. Their motion requires a network of HBs, predominantly between (water or protein) oxygen atoms which are separated to 3 Å or less. Some proteins are flexible, and then HBs break and form continuously. But other proteins (such as the green fluorescent protein, GFP) are rigid and then a large fraction of the HB networks may be visible from its X-ray structure. Yet, to-date there has been no systematic effort in mapping proton wires in proteins. Mrs. Shinobu has done just this, through a computer program that uses

X-ray structures from the Protein Data-Bank (PDB) to divide all HBed atoms in a protein into exclusive clusters, so that in each cluster there is a continuous pathway between any 2 atoms in the cluster, whereas there is no pathway connecting different clusters.

When applied to GFP, the program finds substantially larger clusters than those reported in the literature. Particularly notable is the discovery of a second large internal cluster on the other side of the chromophore than the "active-site cluster" reported before. This cluster is disconnected from the active site, so that the question is what may be its functional role? Our hypothesis is that it functions in executing PT reactions pivotal for the chromophore biosynthesis known to occur after protein folding takes place. There are 4 such PT steps, the last suggested to be extraction of a proton from a bridge carbon of the chromophore to create a carbanion intermediate. We suggest that Thr62, which is located on the new wire, may rotate to pick up this proton and deliver it to the new HB wire, as shown in Figure 4. The delocalization of the proton on this cluster then allows time for completion of the last dehydration step required to form the conjugated system.

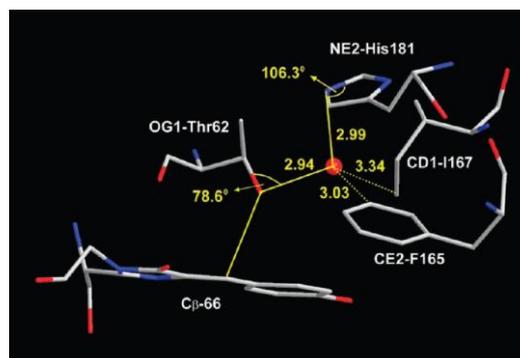


Figure 4: Rotation of Thr62, perhaps together with a migration of a water molecule, are conjectured to play a role in the extraction of a proton from the C-beta carbon of Tyr66, which then becomes part of an extended pi-system of the GFP chromophore.

In human carbonic anhydrase a proton exit pathway frequently discussed is via the rotation of His64. Other pathways are rarely ever discussed. We have found that there are pathways

INDIVIDUAL RESEARCH REPORTS

Noam Agmon

leading up from the "active site caldera", where the Zn^{+2} center resides, to a bunch of carboxylates (Figure 5). These may act to trap a proton from solution and channel it along the surface and into the active site whenever the enzyme operates in the reverse, dehydration direction.

References:

- ❖ A. Shinobu and N. Agmon, J. Phys. Chem. A 113, 7253–7266 (2009).

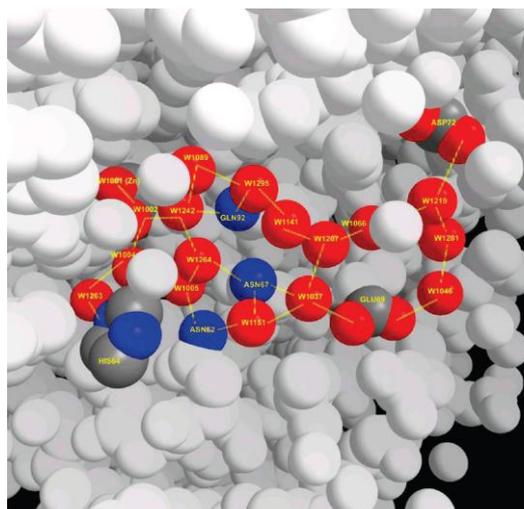


Figure 5: A HB network extends from Tyr66 on the GFP chromophore, via the internalized Glu222 residue all the way to the surface of the barrel-structured GFP.

PROFESSOR AGMON'S GROUP 2005-2009

Name	Status	Presently
Hadas Lapid	MSc	Ph.D. student at Weizmann Inst.
Omer Markovitch	MSc, 2008	Ph.D. student at Weizmann Inst.
Ai Shinobu	MSc	Near graduation
Dr. Soohyung Park	Postdoc 2007-2008	2 nd Postdoc Prof. Arun Yethiraj, Univ. Wisconsin

SCIENTIFIC COLLABORATIONS

Name	Institution
Prof. Dr. Wolfgang Rettig	Humbolt University, Berlin, Germany
Prof. Dan Huppert	Tel-Aviv University, Israel
Prof. Attila Szabo	NIDDK, NIH, Bethesda MD, USA
Dr. Irina Gopich	NIDDK, NIH, Bethesda MD, USA
Prof. Kook-Joe Shin	Seoul National Univ., Seoul, S. Korea
Prof. Gregory A. Voth	Univ. Utah, Salt Lake City UT, USA
Prof. Joel M. Friedman	Yeshiva Univ., Bronx NY, USA
Prof. Huib J. Bakker	FOM Institute for Atomic and Molecular Physics, Amsterdam, Nederland
Dr. Gottfried J. Palm	Univ. Greifswald, Germany

ACTIVE GRANTS

Project	Period	Foundation	Total Grant
Solvation and Migration of Protons	2007-2011	US-Israel Binalational Science Foundation	\$100,000
Water Dynamics and Proton Mobility	2008-2012	Israel Science Foundation	≈ 600,000
Gentner Symposium 2010 (awarded 2008): "Proton Mobility in Chemical and Biological Systems"	2008	Minerva Foundation	€ 61,000

CONFERENCE ORGANIZATION (PAST 5 YEARS)

No.	Conference
1	4th Workshop on Diffusion Assisted Reactions (Org. Guenter Grampp). Schloss Seggau, Leibnitz, Austria, Aug. 21—26, 2004. International Advisory Board.
2	The Fritz Haber Symposium on Biophysical Dynamics (Org. Ronnie Kosloff and Noam Agmon). Mt. Zion Hotel, Jerusalem, March 13—14, 2005.
3	A two-day symposium honoring the retirement of Prof. Menachem Gutman, "Charge Migration in Proteins". Tel-Aviv, Oct. 27—28, 2005. Initiator and Organizing Committee.
4	Research Workshop of the Israel Science Foundation on "Diffusion, Solvation and Transport of Protons in Complex and Biological Systems" (Org. Ehud Pines). Hilton Queen of Sheba Hotel, Eilat, January, 13 - 17, 2008. Organizing Committee.
5	Organizer, 2010 Gentner Symposium on "Proton Mobility in Chemical and Biological Systems". To be held in Ma`agan, Lake of Galilee, Feb 7-12, 2010. Organizing committee: Shy Arkin, Klaus Gerwert and Helmut Grubmüller.

EDITORIAL BOARDS

1. The Israel Journal of Chemistry.
2. PMC Biophysics.

ROI BAER

The 2009 research in Roi Baer's group revolves mainly around developing new density functional and time-dependent density functional theories (DFT and TDDFT). Our methods allow applications of DFT to systems which were previously unattainable, such as charge transfer excitations, structure and properties of radical cations and band electronic structure of solids and large clusters. Some of these works are done in collaboration with Kronik's group in WIS, Daniel Neuhauser (UCLA) and Ulrike Salzner (Bilkent). In 2009 we have developed some fundamental concepts in the description of conical intersection in density functional theory. We have also began in 2009 to study electronic processes in nanocrystals and nanotubes, focusing on multiexciton generation (in collaboration with the Rabani group in TAU).

RESEARCH

GROUND-STATE DEGENERACIES LEAVE RECOGNIZABLE TOPOLOGICAL SCARS IN THE ONE-PARTICLE DENSITY

In Kohn-Sham density functional theory (KS-DFT) a fictitious system of non-interacting particles is constructed having the same ground-state (GS) density as the physical system of interest. A fundamental open question in DFT concerns the ability of an exact KS calculation to spot and characterize the GS degeneracies in the physical system. In this work we provided theoretical evidence suggesting that the GS density, as a function of position on a 2D manifold of param-

eters affecting the external potential, is "topologically scarred" in a distinct way by degeneracies.

We consider 2-fold degeneracies and real Hamiltonians (no magnetic interactions). A basic notion is a 2D manifold of arbitrary parameters, X and Y , that affect the external potential of a particle system (system I). The external potential is a function on the manifold $v(\mathbf{r}; X, Y)$ and by solution of the Schrödinger equation, this potential produces a manifold of GS densities $n(\mathbf{r}; X, Y)$. From the non-crossing rule it follows that in most 2D manifolds 2-fold degeneracies will appear as isolated points and higher degeneracies are practically never seen. A 2-fold dege-

neracy point can be assumed at the origin and polar coordinates used: $X = R \cos \phi$, $Y = R \sin \phi$. The density at the degeneracy is not well defined as there a continuous infinity of densities, corresponding to the infinite ways of combining the degenerate states. When the degeneracy is approached from a given direction ϕ on the manifold the density converges towards a limit function $n(\mathbf{r}; \phi)$ (see Figure 6). This non-analytical behavior on the manifold is "the topological scar".

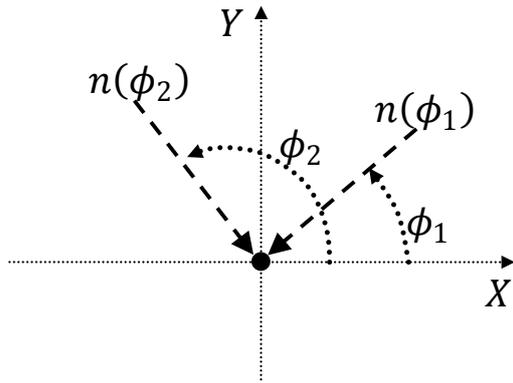


Figure 6: The "topological scar": n_{ϕ_1} and n_{ϕ_2} are particle densities along two distinct paths converging into the same manifold point. If they are different a GS degeneracy exists in system I.

Our paper gives several results concerning these scars. The main conclusion is that the scar will show up in the KS system (system II). We also show that the density itself contains information from which the Berry phase of the system I degeneracy can be reproduced. Furthermore, we argue that the KS Hamiltonian will either be degenerate in the origin or, more likely, will be undefined there (i.e. the KS Hamiltonian itself will have a scar). We also find that in points of non-degeneracy in system I the KS Hamiltonian will either be non-degenerate or will exhibit degeneracy with the density given as a *equal weight ensemble*.

- ❖ R. Baer, "Ground-State Degeneracies Leave Recognizable Topological Scars in the Electronic Density", Phys. Rev. Lett. 104, 073001 (2010).

KOOPMAN'S SPRINGS TO LIFE

The meaning of orbital energies (OOEs) in Kohn-Sham (KS) density functional theory (DFT) is subject to a longstanding controversy. In local, semi-local and hybrid density functionals (DFs) a Koopmans' approach, where OOs approximate negative IPs, is unreliable. We discuss a methodology based on the Baer-Neuhauser-Livshits (BNL) range-separated hybrid DFs for which Koopmans' approach "springs to life". In Figure 7 we show the deviance of negative OOs and SCF/TDDFT energies relative to vertical IPs derived from experiment data for several molecules. The OOs are remarkably close to the negative IPs with typical deviances of ± 0.3 eV even down to IPs of 30 eV, as demonstrated on several molecules. An essential component is the *ab initio* motivated range-parameter tuning procedure, forcing the highest OOE to be exactly equal to the negative first IP.

We developed a theory for the curvature of the energy as a function of fractional occupation numbers to explain some of the results. We now give an expression for the full curvature matrix is

$$C_{mi} \equiv \frac{\partial^2 E_{gs}}{\partial f_m \partial f_i} = \frac{\partial \varepsilon_m}{\partial f_i} = \frac{\partial \varepsilon_i}{\partial f_m}.$$

For clarity, we assume closed shell molecules and we suppress the spin designation for the orbitals $\psi_i \mathbf{r}$ and OOs.

The Hamiltonian \hat{H} is given by

$$\frac{\delta E_{gs}}{\delta \psi_i \mathbf{r}} = \hat{H} \psi_i \mathbf{r}$$

and the density matrix is $\sum_i f_i \psi_i \mathbf{r} \psi_i \mathbf{r}'$. The KS/GKS equations assert

that $\hat{H} \psi_i = \varepsilon_i \psi_i$ and since f_i are *parameters* in

$$\hat{H}, \text{ we have[1]: } \partial \psi_k \mathbf{r} / \partial f_i = \sum_{j \neq k} \omega_{kj}^{-1} A_{jk}^i \psi_j \mathbf{r}$$

where $A_{jk}^i \equiv \langle \psi_j | \partial \hat{H} / \partial f_i | \psi_k \rangle$ and

$\omega_{kj} = \varepsilon_k - \varepsilon_j$; in particular $C_{mi} = A_{mm}^i$. Now,

$\partial \hat{H} / \partial f_i$ not only creates the matrix elements

A_{jk}^i but also depends on them and from this:

$$A_{nm}^i = \sum_{jk} R_{nm\ jk}^{-1} W_{jk\ ii} , \quad (1)$$

where the W matrix corresponds to linear response kernel:

$$W_{jk\ mn} = \iint d^3r d^3r' \left[\begin{array}{c} \left(\frac{1}{|\mathbf{r}-\mathbf{r}'|} + f_{XC}(\mathbf{r},\mathbf{r}') \right) \psi_j(\mathbf{r}) \psi_n(\mathbf{r}') \\ - u(|\mathbf{r}-\mathbf{r}'|) \psi_j(\mathbf{r}') \psi_n(\mathbf{r}) \end{array} \right] \psi_m(\mathbf{r}') \psi_k(\mathbf{r}) \quad (2)$$

This matrix arises from the dependency of the molecular orbitals on the occupation numbers. R^{-1} is the inverse of the total response matrix:

$$R_{jk\ mn} = \delta_{jk\ mn} + \omega_{nm}^{-1} (f_n - f_m) W_{jk\ mn} . \quad (3)$$

In Eq. (2), $f_{XC}(\mathbf{r},\mathbf{r}') = \delta v_{XC}[n](\mathbf{r}) / \delta n(\mathbf{r}')$ is the XC kernel, and $v_{XC}[n](\mathbf{r})$ is the KS or GKS XC potential. In HF theory f_{XC} zero. The function $u(r)$, describing orbital exchange, is: zero in KS theory; $1/r$ in Hartree-Fock theory; and its choice characterizes the kind of GKS theory used: $u(r) = \lambda/r$ (where $0 < \lambda < 1$) for hybrid DFs (in B3LYP $\lambda = 0.2$), and $u(r) = \text{erf}(\gamma r) / r$ for RSH (BNL) DFs (in this latter case $v_{XC}[n](\mathbf{r})$ is dependent on the range-parameter γ as well).

The relation in Eq. (1) is exact but difficult to analyze. To simplify, we neglect the off-diagonal elements of the matrix \bar{R} in Eq. (3), neglecting all $W_{mn\ jk}$ in Eq. (3) except for same-pair interactions, when $mn = kj$. In this case

$$A_{nm}^i = W_{nm\ ii} / R_{mn\ mn} \text{ and in particular:}$$

$$C_{mi} = A_{mm}^i \approx W_{mm\ ii} \quad (4)$$

Applying this result to orbital ε_i itself we find the curvature element $C_{ii} \approx W_{ii\ ii}$ i.e.:

$$C_{ii} \approx \iint d^3r d^3r' \left[\frac{\bar{u}(|\mathbf{r}-\mathbf{r}'|) + f_{XC}(\mathbf{r},\mathbf{r}')}{\psi_i(\mathbf{r})^2 \psi_i(\mathbf{r}')^2} \right], \quad (5)$$

where $\bar{u}(r) = r^{-1} - u(r)$. For HF theory both f_{XC} and $\bar{u}(r)$ vanish and thus $C_{ii} \approx 0$, a result corroborated for $i = N_H$ in calculations.[2-5] For local/semilocal/hybrid DFs, $\bar{u}(r) = 1 - \lambda r^{-1}$, ($\lambda = 0$, local/semilocal and $\lambda = 0.2$, B3LYP) and $f_{XC}(\mathbf{r},\mathbf{r}') \propto \delta(\mathbf{r}-\mathbf{r}')$, leading to $W_{ii\ ii}$ dominated by positive Hartree SR energy for orbital $\psi_i(\mathbf{r})$. This gives significant positive curvature within semilocal DFs as corroborated by numerical calculations.[2-6] We are not aware of calculations for hybrids. Positive curvature grows for localized orbitals as these have large SR. Thus LSDA IPs have larger deviances than B3LYP, which has partial cancelation of SR. In exact KS theory, the nonlocal $f_{XC}(\mathbf{r},\mathbf{r}')$ kernel cancels SR and the curvature should be small. In GKS-RSH theories, which are intermediate between HF and local KS theories, self-interaction is small and the rule that $C_{ii} \approx 0$ holds well as seen in numerical calculations.[2, 4] In BNL curvatures are small, but not exactly zero, thus requiring γ -tuning to have the *initial* slope $\left. \frac{\delta E_{gs}}{\delta f_H} \right|_{f_H=1}$ equal to the *average* slope $-IP_1 = E_{gs}[N] - E_{gs}[N-1]$.

❖ U. Salzner and R. Baer, "Koopmans' springs to life", J. Chem. Phys. 131, 231101-4 (2009).

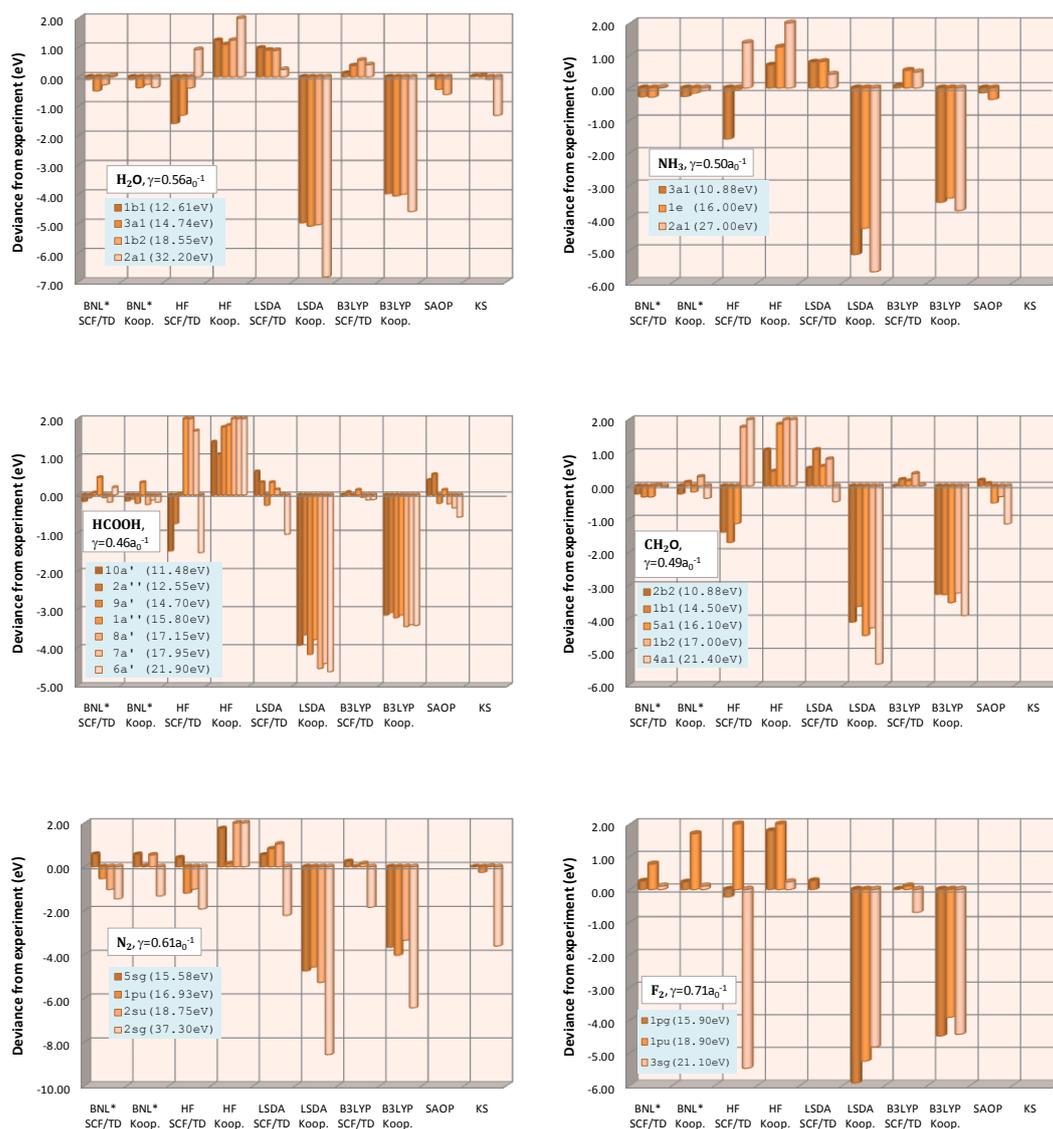


Figure 7: Deviance of negative OOs and SCF/TD energies relative to vertical IPs derived from experiment data for several molecules.

RELIABLE PREDICTION CHARGE-TRANSFER EXCITATIONS IN MOLECULAR COMPLEXES USING TIME-DEPENDENT DENSITY FUNCTIONAL THEORY

Despite its obvious importance, theoretical treatment of the electronic structure aspect of charge transfer excitations has largely been confined to either very small systems where ab-initio wave-function methods can be applied or has relied on empirically calibrated hybrid methods. Typically, excited states in general and optical spectra in particular can be predicted

from first principles using time-dependent density functional theory (TDDFT), which has proven to be a reliable method for studying excited states in broad classes of relatively large systems with good precision. However, it has been shown early on that the adiabatic spatially-local functionals traditionally used within TDDFT do not allow for sufficient accuracy to describe CT excitations. This deficiency, which is not cured by standard hybrid functionals, was attributed to spurious self-interaction and missing derivative discontinuities - two pervasive problems in den-

sity functional theory (DFT) that are intimately related.

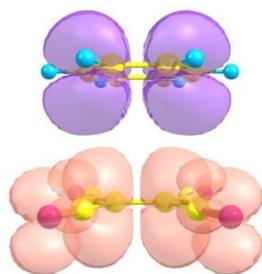


Figure 8: Density difference between the excited state and ground state in the Benzene-TCNE complex, as computed from the excited and ground state Kohn-Sham wave functions. Purple and pink indicate negative and positive densities, respectively, illustrating the charge transfer nature of the excitation.

One way to mitigate the spurious self interaction and to retain a good treatment of correlation is to deploy a range-separated hybrid functional. In this approach, the exchange term in the Kohn Sham energy functional is split into long-range and short-range terms, e.g., via $r^{-1} = r^{-1} \text{erf}(\gamma r) + r^{-1} \text{erfc}(\gamma r)$. The short-range exchange is represented by a local potential derived from the local-density or the generalized gradient approximations. The long-range part is

treated via an “explicit” or “exact” exchange term. If one assumes that an appropriate choice for γ is system independent, its value can be optimized using a molecular training set for optimizing its value. Such semi-empirical approaches, typically with γ in the range of 0.3-0.5 a₀⁻¹, were shown to achieve impressive results for the ground state properties of some classes of systems.

We showed that with the aid of a simple, physically motivated, first principles γ -determining step, range-separated hybrid functionals can be used successfully for quantitative calculation of CT excitation energies. This brings true predictive power to an important area usually considered “too difficult for DFT”. Our approach is tested on complexes formed by an aromatic donor (Ar=benzene, toluene, o-xylene and naphthalene) and the tetracyanoethylene (TCNE) acceptor (see Figure 8), for which optical absorption is available both in gas phase and in solution, as well as on a second set of Ar-TCNE (Ar = anthracene and various meso substituted derivatives) measurements in solution.

Table 1: Excitation energies (eV) and oscillator strengths of several gas phase Ar-TCNE systems: theory and experiment.

Ar	B3LYP		BNL $\gamma=0.5$	BNL γ^*			Exp	
	<i>E</i>	<i>f</i>		γ^*	<i>E</i>	<i>f</i>	<i>E</i>	<i>f</i>
Benzene	2.1	0.03	4.4	0.33	3.8	0.03	3.59	0.02
Toluene	1.8	0.04	4.0	0.32	3.4	0.03	3.36	0.03
o-Xylene	1.5	~0	3.7	0.31	3.0	0.01	3.15	0.05
Naphthalene	0.9	~0	3.3	0.32	2.7	~0	2.60	0.01

Table 2: Excitation energies (eV) in solution of several Ar-TCNE systems: calculation (taking the gas phase result and subtracting 0.32 eV, as discussed in text) and experiment.

Substituent	PBE	B3-LYP	BNL			Exp
			<i>E</i> ($\gamma=0.5$)	γ^*	<i>E</i> ($\gamma=0.3$)	
None	0.9	1.0	2.3	0.31	1.82	1.73
9-cyano	Fail	0.5	2.6	0.30	2.03	2.01
9-chloro	0.9	1.0	2.3	0.31	1.82	1.74
9-carbo-methoxy	0.8	0.9	2.4	0.30	1.84	1.84
9-methyl	1.0	1.1	2.1	0.30	1.71	1.55
9-nitro	0.6	0.9	2.8	0.30	2.12	2.03
9,10-dimethyl	1.3	1.4	2.1	0.30	1.77	1.44
9-formyl	0.8	1.0	2.5	0.30	1.95	1.90
9-formyl 10-chloro	0.8	0.9	2.5	0.30	1.96	1.96

Work done by Tamar Stein (a PhD student in Baer's group). Project is in collaboration with Professor Leor Kronik from the Weizmann Institute.

- ❖ T. Stein, L. Kronik, and R. Baer, "Reliable Prediction of Charge Transfer Excitations in Molecular Complexes Using Time-Dependent Density Functional Theory", *J. Am. Chem. Soc.* 131, 2818-2820 (2009).
- ❖ T. Stein, L. Kronik, and R. Baer, "Prediction of charge-transfer excitations in coumarin-based dyes using a range-separated functional tuned from first principles", *J. Chem. Phys.* 131, 244119-5 (2009).

A NEW GENERALIZED KOHN-SHAM METHOD FOR FUNDAMENTAL BAND-GAPS IN SOLIDS

We developed a method for calculating solid-state ground-state properties and fundamental

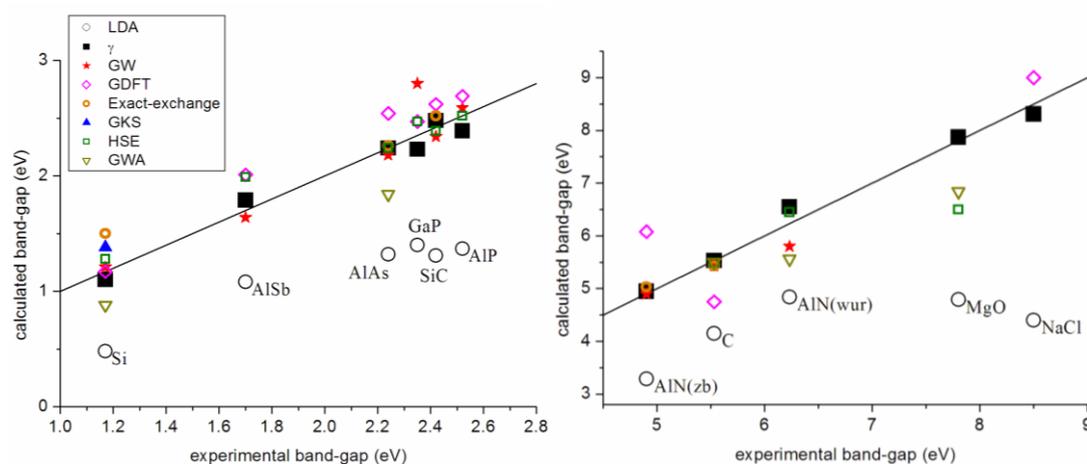


Figure 9: Comparison of calculated vs experimental fundamental band-gaps using different methods. The straight line shows the experimental results. LDA refers to the results obtained using Quantum-ESPRESSO in the local density approximation; γ refers to the results obtained using our modified Quantum-ESPRESSO including our new functional; GW/GWA - results using the GW approximation; GDFT - results using generalized-density-functional theory; Exact-exchange - results using the exact-exchange; GKS - results using the Generalized Kohn-Sham scheme; HSE - results using Heyd-Scuseria-Ernzerhof screened hybrid potential.

Work done with Dr. Helen Eisenberg (Postdoc).

- ❖ H. R. Eisenberg and R. Baer, "A new generalized Kohn-Sham method for fundamental band-gaps in solids", *Phys. Chem. Chem. Phys.* 11, 4674-4680 (2009).

band-gaps using a generalized Kohn-Sham approach combining a local density approximation (LDA) functional with a long-range explicit exchange orbital functional.

We found that when the range parameter is selected according to the formula $\gamma = A/(\epsilon_\infty - \tilde{\epsilon})$ where ϵ_∞ is the optical dielectric constant of the solid and $\tilde{\epsilon} = 0.84$ and $A = 0.216a_0^{-1}$, predictions of the fundamental band-gap close to the experimental values are obtained for a variety of solids of different types. For most solids the range parameter γ is small (i.e. explicit exchange is needed only at long distances) so the predicted values for lattice constants and bulk moduli are similar to those based on conventional LDA calculations. Preliminary calculations on silicon give a general band structure in good agreement with experiment.

THE DELETERIOUS EFFECTS OF LONG-RANGE SELF-REPULSION ON THE DENSITY FUNCTIONAL DESCRIPTION OF O₂ STICKING ON ALUMINUM

Density functional theory (DFT) with semi-local functionals such as the local-density and generalized gradients approximations predicts that the dissociative adsorption of oxygen on Al (111) goes through without a barrier in stark contradiction to experimental findings. This problem motivated our study of the reaction of oxygen colliding with a small aluminum cluster Al₅. We found semilocal functionals predict a minute barrier to sticking, associated with smeared long-range charge transfer from the metal to the oxygen. Hybrid B3LYP predicts a larger barrier while the range-separated the Baer-Neuhauser-Livshits

(BNL, Phys. Chem. Chem. Phys. 9, 2932 (2007)) functional finds a more prominent barrier. BNL predicts short-ranged and more abrupt charge-transfer from the surface to the oxygen. We conclude that spurious self-repulsion inherent in semilocal functionals causes early electron transfer, long-range attraction towards the surface and low reaction barriers for these systems. Our results indicate that the missing DFT barrier for O₂ sticking on Al (111) may be due to spurious self-repulsion.

- ❖ E. Livshits, R. Baer, and R. Kosloff, "Deleterious Effects of Long-Range Self-Repulsion on the Density Functional Description of O-2 Sticking on Aluminum", J. Phys. Chem. A 113, 7521-7527 (2009).

PROFESSOR BAER'S GROUP 2005-2009

Name	Status	Presently
Recca Granot	PhD	Postdoc, HUJI
Dr. Ester Livshits	PhD	Postdoc, HUJI
Shlomit Yacobi	PhD	
Dr. Yair Kurzweil	Postdoc	Second Postdoc, UC Berkeley
Dr. Helen Eisenberg	Postdoc	Current
Omri Buchman	PhD	Current
Adva Baratz	PhD	Current
Tamar Stein	PhD	Current
Dr. Oded Hod	PhD	Senior Lecturer, Tel Aviv University

PROFESSOR BAER'S SCIENTIFIC COLLABORATIONS 2005-2009

Name	Institution
Prof. Leeor Kronik	Weizmann Institute
Prof. Daniel Neuhauser	UCLA
Prof. Eran Rabani	Tel Aviv University
Prof. Ulrike Salzner	Bilkent University
Dr. Nathan Argaman	Nuclear Research Center Negev

ACTIVE GRANTS

Project	Period	Foundation	Total Grant
Near-Field Electron dynamics using time dependent density functional theory	2007-2010	Israel Science Foundation	\$150,000
Density Functional Theory With Correct Long Range Behavior	2006-2009	US-Israel Binational Science Foundation	\$120,000
TDDFT	2009	Army research Lab (ARL, Washington)	\$20,000
Helium diffusion in diamond	2009-2012	Israel Atomic Energy Commission	\$80,000

CONFERENCE ORGANIZATION (PAST 5 YEARS)

No.	Conference
1	The Fritz Haber Symposium on Conductance Yad Hashmona, 2007.
2	Safed Summer school on density functiona theory (Chair: R. Baer, with: E. Rabani and L. Kronik), 2007.
3	2007 Gentner Symposium on "Time dependent density functional theory". Hilton Queen of Sheba, Eilat, Dec. 2007. Chair: R. Baer, with: E. Rabani and L. Kronik.
4	The Fritz Haber Symposium Kibbutz Tsuba, 2009.
5	Victoria Buch Symposium 2010

EDITORIAL BOARDS

Physical Chemistry Chemical Physics (2006).
Annual Reviews of Physical Chemistry (2010-2014)

AVINOAM BEN-SHAUL

My research interests in the last years have focused on several topics involving physic-chemical, statistical-thermodynamic, structural and energetic aspects of biopolymers, bio-molecular assemblies and interactions between them. Most of the work is theoretical, yet most of the projects are closely related to, in some cases, combined with, experimental studies. Among the biopolymers of interest were double stranded (ds) DNA, (single stranded, ss) RNA, naturally unfolded proteins such as MARCKS, and folded proteins – especially cadherins. By macromolecular assemblies we refer here to lipid-protein membranes and viral capsids. We have also studied interactions between the biopolymers and the macromolecular assemblies, e.g., the adsorption of MARCKS onto a mixed, fluid, membrane containing neutral monovalent and multivalent acidic lipids; the packaging of dsDNA within the protein capsid of a bacteriophage, the folding of ssRNA so as to fit the confines of a viral capsid, and the cadherin-mediated adhesion of cells.

The research performed may be termed "multi-scale", in the sense that it ranges from studies involving a single, albeit giant, molecule such as RNA, via the molecular aspects of the interactions between a macromolecule and a macromolecular assembly (e.g., the conformational statistics of the positively charged MARCKS interacting with a mixed, fluid, acidic membrane, DNA confined and (extremely densely) packaged in the capsid of a bacteriophage, or actin polymerization and interaction with a cell membrane), to statistical-thermodynamic models of many molecule systems, such as the exocytosis and budding of enveloped viruses through the cell membrane.

A brief (non exactly chronological) list of the topics studied in the reported period (2002-2009) includes:

- The packaging of dsDNA within the capsid of a λ phage. Calculating the free energy and pressure of the DNA inside the capsid and their change in the course of DNA ejection. (This work was done in collaboration with Bill Gelbart's group of UCLA, partly supported by a BSF grant. Much of the work was done by Shelly Tzlil, a graduate student, now a postdoc in Caltech. Brownian dynamics simulations were done by James Kindt from UCLA). [113,117]
- The mechanism of membrane envelopment of animal viruses and a statistical-Thermodynamic model of the budding process. (With Markus Deserno and Bill Gelbart UCLA, and Shelly Tzlil) [120].
- A Poisson-Boltzmann treatment of the adsorption of charged globular (and rigid) proteins on a membrane containing oppositely charged lipids, and the concomitant clustering of these lipids in the interaction zone. (This work was done in collaboration with Dr Sylvio May, a Minerva postdoc in Jerusalem, and Dr. Daniel Harries during his PHD work). [111, 116, 119, 121, 122]
- Lateral phase transitions of lipid membranes containing charged lipid head groups upon adsorption of oppositely charged macroions. The crucial role of line energy. (With Sylvio May, Daniel Harries and E. C. Mbamala). [115, 127]
- The interaction of a positively charged flexible peptide with a mixed, acidic, fluid membrane: developing a new Monte Carlo (MC) scheme accounting simultaneously for conformational changes of the peptide chain and the lateral mobility of membrane lipids; with emphasis on the enrichment of the adsorption zone by the acidic, especially multivalent, lipids. The MC algorithm enables calculating the free energy, energy, and entropy of interaction as well. (With Shelly Tzlil). [129]
- The binding of the naturally unfolded protein MARCKS to a mixed lipid membranes, with special emphasis on the "electrostatic-switch mechanism". With Shelly Tzlil [134] (See also [132, 133])
- Cadherin-mediated cell-cell adhesion, and the "phase behavior" of binary cell populations. (With the groups of Barry Honig and Larry Shapiro, Columbia University.) [128, 138].
- Modeling the formation of inter-cellular (e.g., adherens) junctions through the coupling of trans-binding between cadherins anchored to apposed cell surfaces, and the lateral (cis) interaction between dimers. (Work in progress, in collaboration with the Columbia group).
- Actin polymerization and the mechanisms of aster-star transition. The relationship of this transition to the biological transition from lamellipodium to a membrane developing filopodia. (Work of the graduate student Yifat Brill-Karnielly. IN collaboration with the group of Anne Bernheim-Grosswasser from Ben-Gurion University.) [130,137].
- The size and shape of viral RNA. Using familiar and newly developed codes we calculated the secondary structures of (numerous) viral and non viral RNA's, and showed that the viral RNA's are "more compact" than non-viral ones; possibly to facilitate their packing in a viral capsid. (In collaboration with Gelbart's group in UCLA, mainly with the graduate student Aron Yoffe.) [136].
- Curvature elasticity of lipid-protein membranes How adsorbed amphipathic peptides affect the spontaneous curvature and bending rigidity of the membrane. (Work of the graduate student, now on the faculty of Hebrew University, Assaf Zemel, in collaboration with Sylvio May from Jena and now North Dakota State University.) [124,126,135].

The section below describes in little more detail a few selected studies. In the section after it you will find a brief "historical overview", summarizing my collaborations and scientific interactions with German and non-German scientists, ending with a few possibly relevant personal notes.

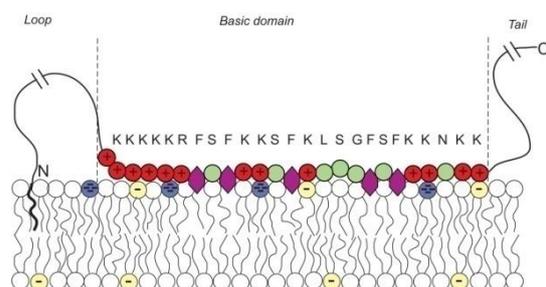


Figure 10: A schematic representation of an adsorbed MARCKS protein. Red and green circles represent charged and neutral amino acids, respectively. Purple hexagons stand for the phenyl groups which tend to insert into the membrane's hydrophobic core. The blue and yellow lipid head-groups represent the tetravalent PIP₂ and monovalent PS lipids, respectively. The amino acid sequence of the basic domain is shown explicitly.

A NON-CHRONOLOGICAL SURVEY OF SEVERAL SELECTED STUDIES

THE "ELECTROSTATIC-SWITCH" MECHANISM: MONTE CARLO STUDY OF MARCKS-MEMBRANE INTERACTION

In a number of papers beginning already in the 1990's we have argued that lipid mobility and redistribution plays a crucial role in the interaction between integral as well as peripheral proteins (and other macromolecules such as DNA) with fluid lipid membranes. We mention here two relatively recent papers [129,134] in which we have studied the interaction of a flexible protein with a mixed, fluid, lipid membrane containing the monovalent acidic PS and the tetra valent acidic lipid PIP₂. In the first study we have focused attention on developing the theory and (the highly non-trivial) simulation algorithm which takes into account, simultaneously, the changes in protein conformation and in membrane local composition. The second paper has been specifically concerned with the interaction of the MARCKS protein with such membrane.

Our goal in this comprehensive theoretical-computational study has been to model the MARCKS electrostatic switch mechanism [134]. Using the Monte Carlo algorithm developed in [129] we have carried out an extensive series of simulations of the intact protein, focusing on the subtle interplay between entropic and energetic contributions to the membrane binding free energy of MARCKS. Using a detailed structural model for the configurational statistics of protein-membrane interaction in the Monte-Carlo simulation scheme, we studied the membrane binding characteristics of MARCKS. This protein comprises a strongly basic (charge $z = +13$) and hydrophobic (five phenylalanines) central domain, with two long flexible chains, one ending with a myristoyl anchor emanating from its ends. We modeled this naturally unfolded protein as a chain of charged, hydrophobic and neutral beads representing the various residues (Figure 10). We considered fluid membranes composed of neutral, monovalent ($z = -1$) and tetravalent PIP₂ ($z = -4$) *laterally mobile* lipids. Based on the simulations we have analyzed the binding characteristics of MARCKS, its phosphorylated isomer ($z = +7$) and some mutants of interest, to different membranes, especially those containing 1% PIP₂. Using Debye-Hückel electrostatic potentials and "semi-empirical" hydrophobic interactions, we found that the major energetic contributions to MARCKS binding are its electrostatic attraction to PIP₂ lipids, and the hydrophobic insertion of phenylalanine and myristoyl anchors. Entropy losses, partly reducing the adsorption free-energy, arise from the lower configurational freedom of the 'end-grafted' side chains, and the "demixing" entropy penalty upon PIP₂ localization. We found that a bound protein typically sequesters ~ 3 -4 PIP₂ lipids, approximately neutralizing its basic domain, and that under physiological conditions protein adsorption is strong and all PIP₂ are bound. The electrostatic switch is triggered by MARCKS phosphorylation, resulting in substantially weaker binding: pro-

teins now leave the membrane, exposing PIP₂ to enzymatic attacks. Our calculations are in good qualitative and quantitative agreement with

available experiments. Illustrative snapshots from such a simulation are shown in Figure 11.

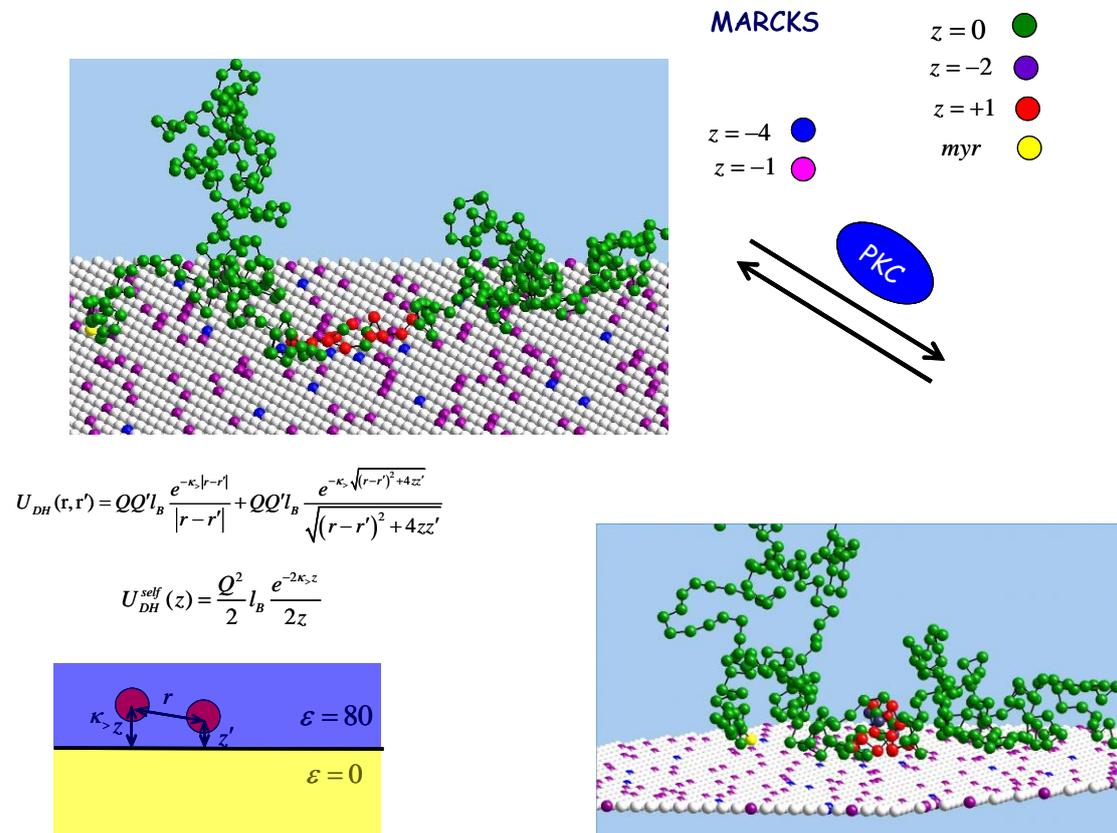


Figure 11: Snapshots from Monte Carlo simulations of MARCKS before (left) and after (right) phosphorylation. Also listed the modified DH potential used.

CADHERIN-MEDIATED CELL-CELL ADHESION, AND THE “PHASE BEHAVIOR” OF BINARY CELL POPULATIONS

A variety of cell-cell adhesion processes are mediated by the binding of cadherin proteins presented on opposing cell surfaces. It has been established in many cases that the identity of the cadherin determines cell-cell adhesive specificity. For example, the differential expression of epithelial (E-) and neural (N-) leads to the separation of the neural tube from the ectoderm in vertebrate embryos. This phenomenon can be mimicked in *in-vitro* cell assays which, under certain conditions, show that cells transfected with N and E cadherin sort out from one another

into separate aggregates. However, aggregation behavior has been shown to depend on expression levels and on the cell growth conditions (e.g shear strengths when the cells are mixed) and there are cases where *in-vitro* cell sorting experiments do not detect homotypic aggregation. It was originally assumed that cadherins were homophilic cell adhesion molecules in the sense that the affinities for the formation of homodimers are significantly higher than for the formation of heterodimers. However, this view has been increasingly questioned, in part because of the inconclusive results obtained from cell aggregation assays.

Detailed experimental studies, involving both molecular structure determinations and the collective behavior of cell mixtures are now in progress at Columbia University (CU) by the groups of Professor Larry Shapiro and Barry Honig. We collaborate closely with these two groups (partly through a joint BSF grant), focusing on correlating the experiments with theory. One aspect of the theoretical research is to relate the microscopic-molecular interactions between pairs of cadherin proteins to cell-cell binding energies and, subsequently, to the “phase behavior” of cell mixtures. The homophilic and heterophilic adhesion, mentioned above, between cells expressing E and N-cadherins provides an excellent, biologically relevant, system for studying such behaviors.

We have formulated a model which enables calculating cell-cell adhesion energies as a function of: the cadherin densities on the surfaces of the apposed cells and the inter-cadherin (trans-binding) energies, which jointly determine the number of inter-cellular trans dimers. Treating cell-cell interactions as analogous to intermolecular interactions, the tendencies of, say, binary (e.g., E and N type) cell mixtures to form mixed (homogeneous) aggregates or to segregate to separate aggregates can then be predicted based on thermodynamic theories of mixing as well as by computer simulations. For the lack of space we shall not go into more details here but suffice in saying that because each cell is covered by numerous (typically many tens of thousands) of cadherin molecules, even tiny differences in molecular adhesion affinities are generally translated into large differences in (e.g., E-E, E-N, N-N) inter-cell adhesion energies. Using our model we have calculated the cell adhesion energies for the N-N, N-E, and E-E pairs and the theoretical predictions are in agreement with the (preliminary) experimental results available so far. In Figure 12 we show images demonstrating the aggregation behavior of a mixture of N-cadherin and E-Cadherin expressing cells. The top panel shows what happens when a population of E-cells labeled by green fluorescing molecules is mixed with another population of E-

cells, labeled red. As expected, the two populations mix randomly to form homogeneously aggregates. Similarly, the second panel from top shows the same behavior for N-cells. On the other hand, using green labels for E-cells and red for N-cells (or vice versa) demonstrate very clear that the different cell populations tend to segregate into distinct aggregates, demonstrating the homophilic character of E-cell and N-cell adhesion. A manuscript summarizing the experimental results and their theoretical has recently been completed [138].

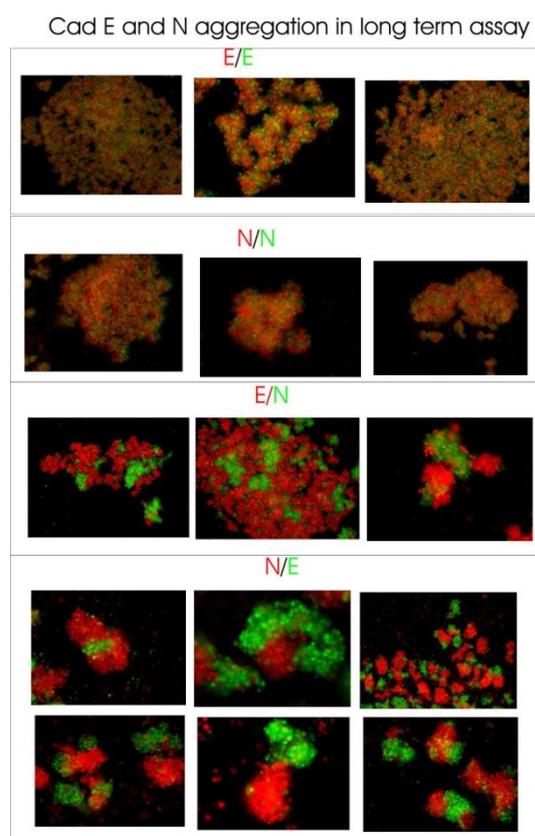


Figure 12: Images demonstrating the aggregation behavior of a mixture of N-cadherin and E-Cadherin expressing cells

ACTIN POLYMERIZATION AND THE ASTER-STAR TRANSITION[130,137]

During cellular migration, regulated actin assembly takes place at the plasma membrane, with continuous disassembly deeper in the cell interior. The actin polymerization at the plasma membrane results in the extension of cellular protrusions in the form of lamellipodia and filopodia. The distinct organization and generation

of filaments in each structure uses a different mechanism to produce mechanical force. In the lamellipodia, the actin filaments organize into a flat 2D branched network, whereas in the filopodia they are assembled into long, parallel, closely packed bundles. Different proteins control the assembly of these structures; in the lamellipodia, the branched nucleation is driven by activation of the Arp2/3 complex by Wiskott-Aldrich syndrome protein family (WASP), followed by filament elongation and barbed-end capping by capping proteins (CP). Formin and Ena/VASP proteins concentrated at the tips of filopodia, enable persistent filament elongation and their successive bundling by fascin. In both structures, the barbed ends (i.e., fast growing end) of actin filaments point toward the plasma membrane.

The PhD work of the graduate student, Yifat Brill-Karniely, is concerned with the dynamic and structural aspects of cell locomotion and, in particular, in the factors determining the structure and energetics of lamellipodia. To this end she has developed a comprehensive 3D dynamic Monte Carlo simulation scheme which includes all the relevant processes which play a role during actin polymerization. Among these, apart from monomer association and dissociation are the processes of branching, capping, and inter-filament binding. In previous reports we have briefly described the results obtained using from the simulations, and a paper describing the model and its predictions is in preparation.

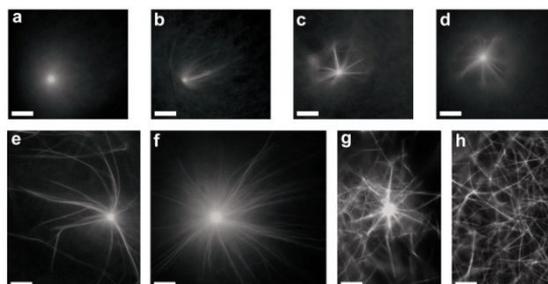


Figure 13: Asters (a and b) growing into stars (c-f) and eventually to networks (g,h) (Experimental results from a manuscript in preparation, by Yaron Ideses, Yifat Brill-Karniely, Lior Haviv, Avinoam Ben-Shaul, and Anne Bernheim-Groswasser).

Actin polymerization in vitro is extensively studied in the group of Anne Berenheim in Ben-Gurion University. We closely collaborate with this group. One phenomenon, resembling the transition from lamellipodia to filopodia, is the transition observed in actin containing solutions from a dense (nearly spherical) actin aggregates termed 'aster', to a 'star' like structure where bundles of several bound filaments emanate from the aggregate's (aster) core. Figure 13 shows electron micrographs illustrating the aster-star transition.

To explain the aster-to-star transition we have formulated a simple theoretical model based on the idea that two energetic factors determine the diameter of the bundles: the bending energy associated with bringing two (and later additional) filaments toward each other, and the cohesive energy gained by the fascin proteins which link the filaments together. The model also assumes that the onset of bundling takes place when filament branching slows down, so that the filaments are barely branched and therefore, without interference due to excluded volume interactions, can bend and link as linear semi-flexible polymers, as illustrated in Figure 14.

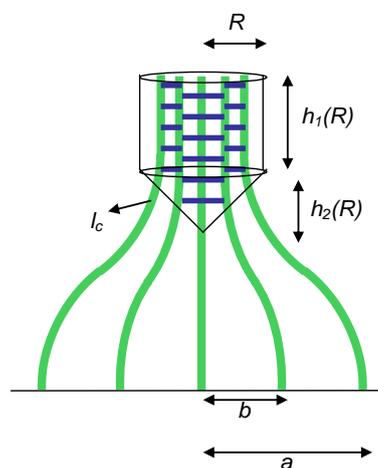


Figure 14: Schematic illustration of filament bundling. Bundling is favored by the energy gained through fascin linking and opposed by filament bending. The optimal bundle diameter is determined by the balance of these two energies and the surface energy of the bundle.

THE SIZE AND SHAPE OF VIRAL RNA

In close collaboration with the group of Professor William Gelbart of the chemistry department at UCLA, and especially his Graduate student Aron Yoffe we are studying, theoretically, the size and shape characteristics of viral RNA, as distinguished from non viral RNA and “random” RNA. Light scattering and other experiments are carried out at UCLA laboratories.

We have recently completed a manuscript summarizing the most comprehensive series of RNA structure calculations which Aron has carried out during the last two years or so. The main goal here was to examine our hypothesis that the dimensions (as measured, for instance, by the radius of gyration) of viral RNA are spatially smaller than those of equally long sequences of non-viral RNA.

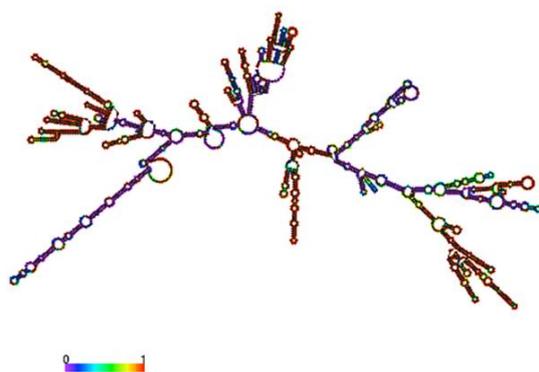


Figure 15: Predicted secondary structure of the BMV3 RNA. The colors describe the relative stability of the given base pair. Highly probable base-pairs (encountered in the most stable structures) are red, least probable are blue.

Our principal theoretical prediction in this work is that the radius of gyration, R_g , of the folded RNA (which resembles a branch polymer) should scale with the square-root of the quantity known as the MLD=maximum ladder distance. (The “ladder distance” measures the number of base-pair “rungs” crossed along the path from one point to another along the RNA backbone). Namely,

$$R_g \approx MLD^{1/2} \approx (N^{0.7})^{1/2} \approx N^{0.35}$$

where N is the number of bases comprising the RNA. The second scaling relation was predicted theoretically by Bundschuh and Wha (Phys. Rev. E. 65, 041903 (2002)). The validity of these relationships should be examined based on experiments which are now in progress. Their qualitative predictions regarding RNA structure are obviously reasonable.

In Figure 15 we show two typical secondary structures of RNA, corresponding to a random and an equally long viral RNA sequence. The maximum ladder path corresponding to the two structures is marked by the dashed curves. The viral RNA is clearly more compact than the non-viral one.

We are also studying other issues pertaining to RNA structure (e.g., the spatial proximity of the two ends of a linear, folded, RNA). Progress on this and other questions will be reported next year.

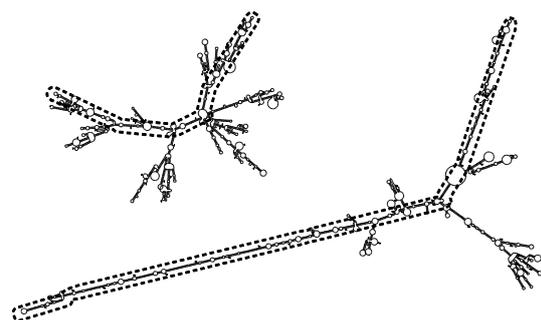


Figure 16: Viral CCMV -RNA1 (top) and a “typical-looking” random ssRNA of the same length (bottom). Note that the secondary structure of the random ssRNA appears to be relatively extended, while that of the viral ssRNA appears to be relatively more compact. This difference in “extendedness” translates into a difference in 3D size.

COLLABORATIONS, HISTORY ETC.

My group, by my choice, has always been small, consisting usually of 2-5, fortunately always excellent, students or postdocs. Exactly seven years ago I started to deal with a severe health problem, and hence decided to stop accepting new students. Presently I have only one graduate student, Yifat Brill-Karnielly, whose thesis is nearly complete. She was offered a postdoctoral position in the group of Daan Frenkel in Cambridge

UK starting summer 2009. Notwithstanding the obstacles of the last seven years we (i.e., me and my students and collaborators) have managed to keep a reasonable level and pace of scientific activity, to a large extent via close collaborations with my colleagues abroad, especially Professors Bill Gelbart from UCLA and Barry Honig from Columbia University, New York. I keep close research ties with other colleagues abroad, including for example Professor Erich Sackmann and Joachim Rädler from Munich.

While the university and the center provide important administrative and system support, the actual funding of the research (which for my group is rather modest) has been provided by a (constant) support from two competitive granting agencies:— the Israel Science Foundation (ISF) and the US-Israel Binational Science Foundation (BSF). I did not apply to other agencies.

I should perhaps mention that many years ago I had very tight research relations with German scientists; primarily Professors Karl Kompa (with whom together with professors Y. Hass and R. D. Levine we have published in 1980 a book named "Lasers and Chemical Change") and with Dr. Frank Reberndt with whom I have published several (in my opinion nice and important) papers. In fact, I was among the first Minerva fellows in Germany, 1972-1974, postdoc-ing in the Lehrstuhl für Theoretische Chemie in the TUM, headed by Professor L. Hofacker and later mainly with Professor Karl Kompa in the MPI for quantum Optics in Garching. Till around 1985 I kept scientific ties with Professors Kompa and Reberndt, working on multiphoton ionization and surface reaction kinetics. I keep friendly ties with all my colleagues from this period, but these are mainly social now, because starting around 1980 my research has taken a turn focusing on self assembling and biophysical systems. On the other hand starting around this time I kept close scientific connections with Professor Erich Sackmann, through many short and long mutual visits, as well as with several young German scientists.

My closest collaboration with a German scientist has been with Dr. Sylvio May from Jena who spent here two years as a Minerva postdoctoral fellow, and many shorter visits both before and after this postdoctoral period. Our collaboration has started already when he was a graduate student and intensified later during his two years stay in Jerusalem. This collaboration has yielded twenty joint articles on several different topics (published between 1995 and 2007), and has been most beneficial for both of us. Sylvio is now a professor in a North Dakota State University. Other young German scientists with whom I collaborated are Professors Joachim Rädler; we have published a joint theoretical-experimental paper in which we have demonstrated for the first time the phenomenon of "counterion release" upon the formation of a condensed phase of oppositely charged macroions [107]. Another fruitful collaboration has been with Dr. Marcus Deserno from Mainz (now a professor at Carnegie Mellon University), on the issue of viral budding [123].

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PROFESSORS BEN-SHAUL'S GROUP (PAST 5 YEARS)

Name	Status	Presently
Dr. Shelly Tzlil	PhD	Postdoc in the group of David Tirrell; Caltech
Yifat Brill-Karniely	PhD	Near graduation; Will leave for postdoc in Cambridge UK
Aron Yoffe	Visiting student	PhD in UCLA
Dr. Vladimir Teif	Visitor from Belarus	Heidelberg

ACTIVE GRANTS

Project	Period	Foundation	Total Grant
Cadherin Mediated Cell-Cell Adhesion	2007-2011	US-Israel Binational Science Foundation	\$80,000
Biopolymers Interacting with Mobile Surface Charges	2006-2010	Israel Science Foundation	~\$150,000

EDITORIAL BOARDS, PRIZES

- Chemistry and Physics of Lipids
- PMC (PhyMathCentral) Biophysics
- Landau Prize for "Physics of Membranes, Polymers and Biomaterials".

VICTORIA BUCH 1954-2009

Professor Buch has passed away on 21 June 2009 following a heroic struggle with a deadly cancer disease. On that day the director of the center sent the following mail to the center members, Beirat and friends:

Friends,

I have sad news. A dear friend, teacher, colleague, and wonderful human being, Professor Victoria Buch, has passed away today, after a long struggle with a fatal disease.

I want to write a few personal words about the Victoria I will miss very much. Victoria the "real" person. Very few are, in my view. I see in Victoria a real scientist. She did not follow trendy puffs of wind; she chose instead to grapple with the more basic, deep and difficult scientific questions of chemistry. She had the "nose" for asking those really interesting fundamental questions in her field and the creativity to develop theoretical and computational methods to answer them. Some highlights of Victoria's career include the brilliant diffusion Monte Carlo method she developed for rigid bodies and her many important landmark works on the structure and spectroscopy of ice and water, their surfaces and their chemistry.

Victoria is a real human being. Yes, she was too often late to here and unintentionally absent from there... sometimes totally forgetting her schedule... or where she left her cell-phone... But I knew: this is just scratching the surface. Actually, I always felt this "absent-minded-professor" was much more in touch with reality, connected to this world, than I will ever be! This is because Victoria's eyes and heart were open to see and feel the harsh events around us here in Israel. She made no concessions, no compromise, always true to her conscious. She fiercely demanded and fought for justice and compassion in times few have the patience and integrity to rise above their anger to do so.

Victoria willingly paid a high price for her social and political activities. Few would be able to stay so scientifically prolific, highly cited and internationally acknowledged as Victoria while concurrently devoting a huge portion of their time and patience to actively help the weak, the vulnerable and the suffering. Indeed, Victoria was constantly busy demonstrating, blockade-watching, writing letters, publishing petitions and lecturing about these "real world" matters! Some people in our department may have bitterly disagreed with her views and actions. But I am sure they were secretly impressed by her sincere and pure intentions realizing she was constantly searching for the 'good thing to do'. (And perhaps that made them even more cross...)

I was not a student of Victoria. Never took a formal course or class with her. But I learned a lot from her – just by watching. And she was a great teacher!

It is so sad for me that a beautiful person as Victoria was snatched from my world, so suddenly, so brutally and so much too early!

Roi Baer, 20/6/2009

On 9 May 2010 a symposium in her memory, with participation of her scientific friends and research collaborators was held in the Hebrew University, organized by Professor Baer. The 2010 Gordon conference on water and aqueous solutions (August 8-13), organized by Pavel Jungwirth and Victoria

Buch will include a session held in her memory. A Victoria Buch Memorial volume will be published next year in the Journal of Physical Chemistry Part A.

Despite her deteriorating health condition, Victoria Buch worked relentlessly, practically up to the very last day, on finalizing her last scientific contributions. These were published during the years 2008-2010, as listed below:

1. S. Bauerecker, P. Ulbig, V. Buch, L. Vrbka, and P. Jungwirth, "Monitoring ice nucleation in pure and salty water via high-speed imaging and computer simulations", *J. Phys. Chem. C* **112**, 7631-7636 (2008).
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3. V. Buch, H. Groenzin, I. Lit, M. J. Shultz, and E. Tosatti, "Proton order in the ice crystal surface", *Proc. Natl. Acad. Sci. U. S. A.* **105**, 5969-5974 (2008).
4. A. D. Hammerich and V. Buch, "An alternative near-neighbor definition of hydrogen bonding in water", *J. Chem. Phys.* **128**, - (2008).
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ROBERT B. GERBER

The main research activities of our group in 2009 have been in: mechanisms and dynamics of atmospherically-important reactions; vibrational spectroscopy of biological molecules; interactions of saccharides with water molecules and with ions; lifetimes, kinetic stability and other properties of new noble-gas molecules. A brief description of several research highlights obtained or published by our group in 2009 follows here.

SCIENTIFIC PROJECTS

IONIZATION OF N_2O_4 IN CONTACT WITH WATER: MECHANISM, TIMESCALES AND ATMOSPHERIC SIGNIFICANCE

The hydrolysis of NO_x species, in particular of N_2O_4 , is a process of major atmospheric interest. A kinetic mechanism for the hydrolysis has been proposed by B.J. Finlayson-Pitts, and involves among other points the assumption that cleaves N_2O_4 into the ion pair $(NO^+)(NO_3^-)$, which are involved in subsequent reactions. However, no macroscopic evidence for this assumption is available. Simulations done by Yifat Miller, then a Ph.D. student in our group, in cooperation with Professor Finlayson-Pitts and her experimental group, give strong support for the assumed ionization, and provide quantitative data on the process and the microscopic mechanism involved.

The simulations used N_2O_4 on water clusters as a model system. Direct dynamics calculations were used, employing MP2 potentials “on the fly”. The *ab initio* MP2 method has been demonstrated to be very reliable for water clusters, hence the importance of using it in the “on the fly” dynamics. The results show that a single water molecule suffices to induce ion pair formation at 300K, the process taking place on a picoseconds timescale. The presence of several additional water molecules accelerates the process to a femtosecond timescale.

A referee report on the paper presenting this work hailed it as a very important result. This paper^(a) was selected by the Editor as a Cover Article of the issue in JACS. Figure 17 from the paper depicts the mechanism of the process, as obtained from the simulation.

(a) Y. Miller, B.J. Finlayson-Pitts and R.B. Geber, Ionization of N_2O_4 in Contact with Water: Mechanism, Timescales and Atmospheric Implications, *J. Am. Chem. Soc.* **131**, 12180-85 (2009). (Cover Article)

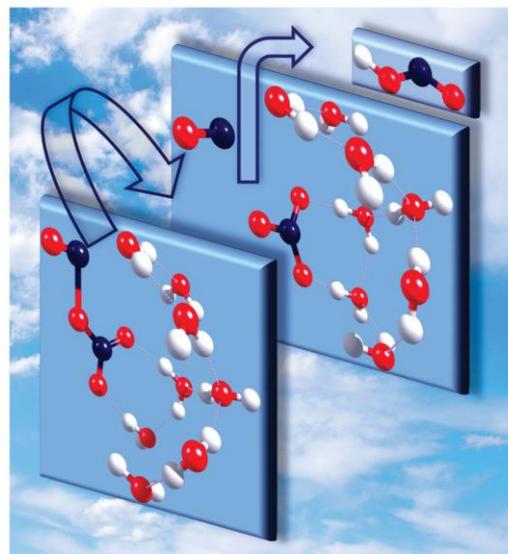


Figure 17: Mechanism of the Hydrolysis of asymmetric N_2O_4 at a Water Cluster.

CATALYTIC ROLE FOR WATER IN THE ATMOSPHERIC PRODUCTION OF CLNO

Computational studies by B. Njegic, a postdoc in our group, show that a single water molecule catalyzes the production of ClNO, a major source of atomic chlorine in the atmosphere, from $ONONO_2$ and HCl. These results provide a microscopic interpretation for experimental results by Finlayson-Pitts and coworkers, showing that production of ClNO from N_2O_4 and HCl is greatly accelerated at water films. The results point to a new key mechanism for the production of Cl in the atmosphere, and already had an impact in the atmospheric chemistry community. Snapshots from “on the fly” MP2 simulations of the process are shown in Figure 18.

A paper^(b) describing these results, published in PNAS, was selected as Cover Article for the issue.

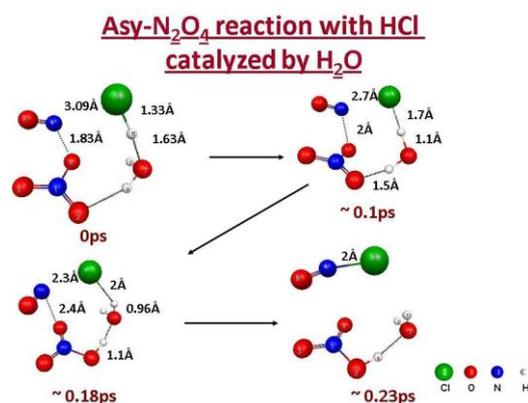


Figure 18: Snapshots showing the formation of ClNO from ONONO₂ in a cluster with a single water molecule.

(b) J.D. Raff, B. Njagic, W.L. Chang, M.S. Gordon, D. Dabdub, R.B. Geber and B.J. Finlayson-Pitts, "Surface-Mediated Reactions of Nitrogen Oxides with Hydrogen Chloride: Indoor and Outdoor Chlorine Activation", Proc. Nat. Acad. Sci. 106, 13647-54 (2009). (Cover Article)

PROPERTIES OF NEW NOBLE-GAS COMPOUNDS

The chemical bonding, kinetic stability and decomposition pathways and other properties of new noble-gas compounds continue to fascinate us, and to stimulate our research, mostly in cooperation with experimental groups in the field. A result on an important issue that received much attention so far is on the lifetimes of new noble gas compounds: Combining multi-reference methods with Transition State Theory, interesting results were obtained for HXeOH and HXeOXeOH, two compounds made of Xe and water(1). A spectroscopic experimental/theoretical study on xenon hydrides established that there is a direct H-Xe bond in these molecules(2). The paper describing this result was selected by the Editor of J. Chem. Phys. as one of the research highlight papers for 2009.(2) Another article is a review paper co-authored by RBG and two of the leading experimentalists in the field(3). This paper describes the nature of bonding and provides insights into properties of the noble-gas hydrides, a new family of compounds in the development of which the authors have played a key role.

(1) U. Tsvion and R. B. Geber, Lifetimes of Compounds Made of Noble-Gas Atoms with Water, Chem. Phys. Lett. 482, 30-33 (2009).

(2) V.I. Feldman, A.V. Kobzareno, I.A. Baranova, A.V. Danchenko, F.O. Sukhov, E. Tsvion and R.B. Geber, Direct Visualization of the H-Xe Bond in Xenon Hydrides: Xenon Isotopic Shift in the IR Spectra, J. Phys. (Communication), 131, Art. 151101/1-3 (2009). (Editor's choice for a JPC Research Highlight).

(3) L. Khriachtchev, M. Räsänen and R.B. Geber, Noble-Gas Hydrides: New Chemistry at Low Temperatures, Acc. Chem. Res. 42, 183-191 (2009).

SEPARATION OF IONS IN SUGAR-SALT-WATER COMPLEXES

This work is part of a project on processes in saccharides, potentially relevant to production of biofuels. This project was conceived and developed jointly with the late Professor Victoria Buch. Intense cooperation with her continued to the very last days of her life, and her ideas, insights and dedication continue to be a source of inspiration.

The question of separation of salt molecules into ions in saccharides is of technological as well as fundamental interest. This was investigated by MD simulations using a novel force field (DL-POLY), as well as Car-Parrinello simulations with BLYP-type interactions. Insight from the two types of simulations helps in identifying simulation results that can be relied upon as representing physical reality.

It was found that the salt KNO₃ does not separate into ions in the glucose-KNO₃ complex, even at high temperatures ($T \gg 300\text{K}$). On the other hand, with the addition of $n \geq 3$ water molecules, ion separation takes place, and the K⁺ and are each locally solvated, the anion by both water molecules and a sugar OH group. Entropy is a key factor in deriving the separation. Snapshots of the separation process are shown in

Figure 19. A paper presenting these results was published recently in PCCP.(c)

Ion Separation Dynamics in Glucose $\text{KNO}_3-(\text{H}_2\text{O})_3$

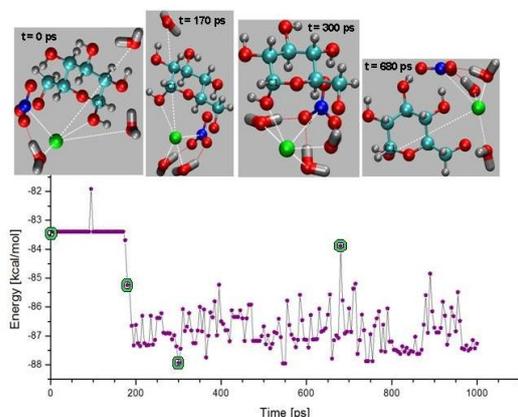


Figure 19: Snapshots showing the separation of K^+ and in Glucose-KNO $_3$ -(H $_2$ O) $_3$

(c) M. Pinciu, B. Brauer, R.B. Gerber and V. Buch, Sugar-Salt and Sugar-Salt-Water Complexes: Structure and Dynamics of Glucose-KNO $_3$ -(H $_2$ O) $_n$, Phys. Chem. Chem. Phys. **12**, 3550-58 (2010). (Themed issue: Biomolecular Structures: From Isolated Molecules to Living Cells”.

VIBRATIONAL STATES AND DYNAMICS OF SMALL WATER CLUSTERS

Small water clusters are systems of interest to our group, especially as model systems for atmospherically-relevant systems. Work is in progress, in cooperation with experiments by the group of Professor B. Abel (Leipzig) on the dissociation dynamics of (H $_2$ O) $_n$ clusters, following OH($\nu=1$) stretching excitation.

❖ O. Link, E. Vöhringer-Martinez, E. Lungovoj, X. Liu, K. Seifermann, M. Faubel, H. Grubmüller, R.B. Gerber, Y. Miller and B. Abel, Ultrafast Phase Transitions in Metastable Water Near Liquid Interfaces, Faraday Discuss. **141**, 67-69 (2009).

ACADEMIC ACTIVITIES, 2005-2009

- (1) Member of the Scientific Committee of the Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague (from 2005).
- (2) Member of the Editorial Advisory Board, Journal of Chemical Physics, 2001-2004.
- (3) Member of the Editorial Advisory Board, Chemical Physics (continuing).
- (4) Member of the Editorial Board of Computational Material Science (continuing).

ACTIVE GRANTS

Granting Agency	Period	Amount
DFG – SFB 450	Jan 2002 – Dec 2009	Euro 360,180
Isr. Sci. Found. (ISF)	Oct 2002 – Sept 2003	NIS 34,000
US-Israel Science Foundation (BSF)	Sept 2005 – Aug 2009	\$ 81,900
Govt. Tech. Projects	June 2006 – Jan 2010	NIS 300,000
Govt. Tech. Projects	Oct 2006 – Feb 2009	NIS 609,000
Isr. Sci. Found. (ISF)	Oct 2008 – Sept 2009	NIS 172,000
Govt. Tech. Projects	Sept 2008 – Sept 2009	NIS 150,000
Govt. Tech. Projects	Feb 2009 – Jan 2010	NIS 650,000
Govt. Tech. Projects DARPA (USA)	Jan 2009 – Dec 2009	\$ 500,000

PROFESSOR GERBER'S GROUP 2009

Name	Status	Presently
Dr. Adesokan, A.A	PhD	Postdoc, Harvard University
Ansbacher, T.,	M.Sc	
Dr. Bihary, Z.	PhD	Research Inst. in Hungary
Dr. Cohen, A.	PhD	Postdoc, Duke University
Dr. Eshet, H.	MSc	Postdoc
Dr. Miller, Y.	PhD	Postdoc, NIH
Dr. Niv, M.Y.	PhD	Senior Lecturer, Faculty of Agriculture, Hebrew University
Dr. Shemesh, D.	PhD	Postdoc Munich Univ.
Dr. Brown, E.C.	Postdoc	Assistant Professor, Loyola University, Chicago
Dr. Kamboures, M.	Postdoc	State of California, Atmospheric Agency
Professor Sheng, L.,	Postdoc	University of Harbin, China
Dr. Brauer B	Postdoc	Current member of the group
Goldstein, M.,	PhD	Current member of the group
Hirshberg, B.	Undergraduate	Current member of the group
Knaanie, R.,	PhD	Current member of the group
Lignell, H.	PhD	co-advised by Prof. M. Räsänen, Current member of the group
Dr. Njegic, B.	Postdoc	Current member of the group
Ofir-Smilovici, M.	PhD	Current member of the group
Pele, L.	PhD	Current member of the group
Pincu, M.	PhD	Current member of the group
Sagi, E.	MSc	Current member of the group
Dr. Sebek, J	Postdoc	Current member of the group
Shahar, A.	MSc	Current member of the group
Dr. Steinberg, M.	Postdoc	Current member of the group
Dr. Suwan, I.,	Postdoc	Current member of the group
Tsivion, E.	PhD	Current member of the group
Zax, H	Undergraduate	Current member of the group
Zmiri, L	MSc	Current member of the group

AWARDS AND HONORS 2005-2009

- ❖ Prize of the Israel Chemical Society for 2004.
- ❖ Medal of the Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague, 2006.
- ❖ Foreign member of the Finnish Academy of Sciences and Letters, elected 2007.
- ❖ Festschrift for R.B. Geber, special issue of J. Phys. Chem., edited by A.B. McCoy, A. I. Krylov and V. Buch (in preparation, to appear in 2009).
- ❖ Editorial advisory board, Chemical Physics (continuing).
- ❖ Editorial board of Computational Material Science (continuing).

DANIEL HARRIES

In the past year we have continued to focus our study on the way macromolecules interact in solution. We are interested in a wide variety of macromolecules, most of which have biological importance. These can be large protein molecules and their aggregates, lipid membranes, DNA, and their combined complexes as found in viral particles. The main theme is to analyze macromolecular interactions in terms of the mediating environment, to achieve a unified description of complex crowded and confined solutions, such as can be expected to be found in living cells. In the following we describe our main studies that were completed over the past year.

CHOLESTEROL ORDERING IN LIPID MEMBRANES

An essential component of mammalian cell membranes, cholesterol is known to be critical for membrane organization, dynamics, and function. The nonuniform distribution of cholesterol between cellular organelles, lipid membrane compartments, and even between leaflets of the same bilayer, highlights cholesterol's role in influencing the biophysical properties of a fluid lipid matrix and in the stabilization and function of membrane proteins through specific interactions. The great variability found in the concentration of cholesterol among various cells and between the plasma membrane and the variety of membranes of other cellular organelles underscores the importance of tightly regulated cholesterol content for proper function at the subcellular level. In fact, inborn errors of cholesterol synthesis lead to major developmental abnormalities, and conversely, an excess of cholesterol is widely acknowledged as detrimental.

We performed molecular dynamics (MD) simulations of hydrated bilayers containing mixtures of dimyristoylphosphatidylcholine (DMPC) and cholesterol at various ratios, to study the effect of cholesterol concentration on its orientation, and

to characterize the link between cholesterol tilt and overall phospholipid membrane organization. The simulations show a substantial probability for cholesterol molecules to transiently orient perpendicular to the bilayer normal, and suggest that cholesterol tilt may be an important factor for inducing membrane ordering. In particular, we find that as cholesterol concentration increases (1-40% cholesterol) the average cholesterol orientation changes in a manner strongly (anti)correlated with the variation in membrane thickness. Furthermore, cholesterol orientation is found to be determined by the aligning force exerted by other cholesterol molecules, see Figure 20. To quantify this aligning field, we analyzed cholesterol orientation using, to our knowledge, the first estimates of the cholesterol tilt modulus χ from MD simulations. Our calculations suggest that the aligning field that determines χ is indeed strongly linked to sterol composition. This empirical parameter (χ) should therefore become a useful quantitative measure to describe cholesterol interaction with other lipids in bilayers, particularly in various coarse-grained force fields.

❖ George Khelashvili, Georg Pabst, and Daniel Harries J. Phys. Chem B (in press, 2010)

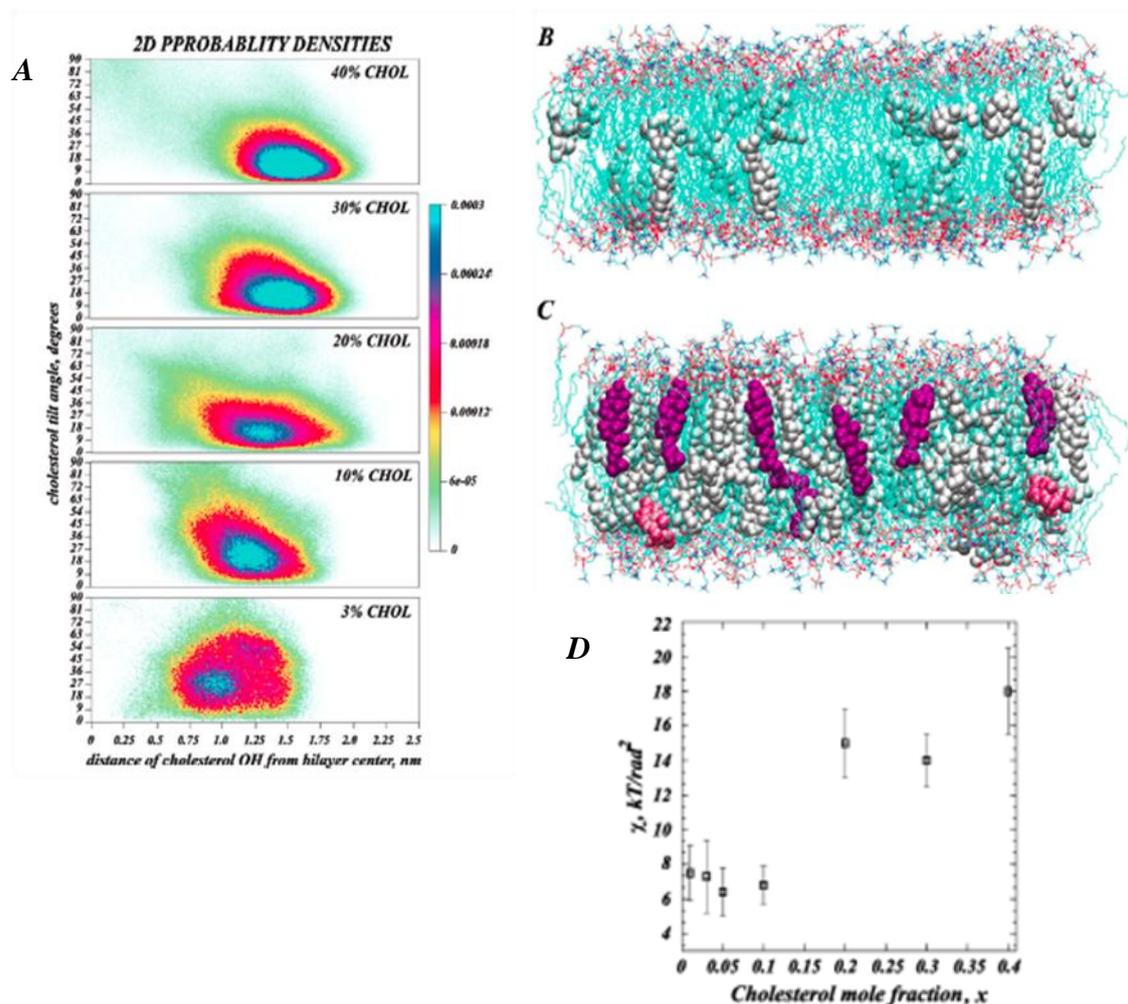


Figure 20: Cholesterol in membranes transition from a broad orientational distribution at low cholesterol mole fractions to high cholesterol fractions. This change in orientation can be seen in the probability distributions in A as a function of depth in the membrane and tilt angle, and also in the simulation snapshots in panels B (low cholesterol content of 3%) and D (high cholesterol content of 30%). These orientational changes can be translated to a stronger tilt modulus for high cholesterol content membranes. This modulus is shown in panel D to transition sharply to a higher value at the concentration regime for which the lipid membrane undergoes a first order transition from lipid disordered to lipid ordered phases.

THE EFFECT OF COSOLUTES ON PEPTIDE FOLDING AND AMYLOID AGGREGATION OF A MODEL PEPTIDE

Living cells have developed multiple strategies to ensure that correct protein folding occurs even under substantial environmental stresses. Among the most widely employed methods to counteract external osmotic pressure is the use of small cosolutes called osmolytes. The exact mechanism of macromolecular stabilization by osmolytes is still largely unknown, but it has been recognized that solutes stabilizing the native state of proteins (protective osmolytes) tend

to be preferentially excluded from protein-water interfaces.

Molecular crowding due to excluded volume interactions has been widely invoked to explain how osmolytes can drive protein stability. For example, it was shown that high fractional volume occupancy of crowding agents, such as soluble polymers, significantly shifts the non-native to folded thermodynamic equilibrium toward the more compact native states. This effect was shown to be related to the restriction of protein conformations to allow larger free volume for osmolytes, thereby destabilizing the unfolded state with respect to the native conformation.

However, such molecular crowding mechanisms that are based on steric interactions and are entropic in nature do not usually consider the possibility of enthalpic contributions that may be mediated by the aqueous solution.

We have focused on the effects of various molecularly small osmolytes on the stability of a model 16-residue peptide that can fold to a β -hairpin structure. In aqueous solutions and at neutral pH, this peptide folds in an endothermic, entropically driven process. Surprisingly, in contrast to the crowding mechanism, polyol and sugar osmolytes act to drive further folding primarily through diminishing the enthalpic loss with concomitant reduction in the favorable entropic gain for folding. Although the osmolyte effect is strongly enthalpic, the action of different osmolytes correlates with their size, as also expected for crowding. Our results further suggest that osmolytes act indirectly by altering the solvating environment, rather than by interacting directly with the peptide.

This previously unreported mechanism for osmolyte action on peptide folding highlights the possible importance of water structuring forces in addition to the entropic crowding effects in determining protein stabilization by osmolytes. Such insights should provide a better understanding of the variety of physical forces by which protective osmolytes stabilize proteins in biologically realistic solutions.

We have also been interested in the action of osmolytes on Amyloid fiber formation that is a specific form of protein aggregation, often resulting from the misfolding of native proteins. Recent experiments showed a reduction in fibrillation halftimes in the presence of inert cosolutes used to model the crowded environment of the cell. This effect has previously been accounted for by considering the large volume excluded by inert cellular solutes, sometimes termed “macromolecular crowding”. We studied a synthetic 16 amino-acid peptide that forms amyloid fibrils under certain solution conditions. Using Circular Dichroism spectroscopy (CD) we found that the more compact β -hairpin confor-

mation of the monomeric peptide is stabilized in the presence of inert cosolutes, and that stabilization is linear in both solute volume and concentration, as also predicted by molecular crowding models. In contrast, the fibrillation process, as followed by ThT fluorescence, cryo-electron microscopy, and CD spectroscopy, remained unaffected by soluble polyethylene glycols of different molecular weights. Surprisingly, however, the smaller polyols glycerol and sorbitol acted to increase the lag time for fibril formation and the amount of peptide that had undergone fibrillation. This example highlights the importance of other forces beyond the purely entropic mechanism of solute excluded volume that may contribute to the cosolute effects acting on amyloid formation.

- ❖ Regina Politi, Shahar Sukenik, Daniel Harries, in collaboration with Lior Zisserman, Dganit Danino (Technion), and Assaf Friedler (HUJ)

DEPLETION FORCES DRIVE POLYMER-LIKE SELF-ASSEMBLY IN VIBROFLUIDIZED GRANULAR MATERIALS

Ranging from nano- to granular-scales, control of particle assembly can be achieved by limiting the available free space, for example by increasing the concentration of particles (crowding) or through their restriction to 2D environments. It is unclear, however, if self-assembly principles governing thermally equilibrated molecules can also apply to mechanically excited macroscopic particles in nonequilibrium steady-state. We have shown that low densities of vibrofluidized steel rods, when crowded by high densities of spheres and confined to quasi-2D planes, can self-assemble into linear polymer-like structures (Figure 21). Our 2D Monte Carlo simulations show similar finite sized aggregates in thermally equilibrated binary mixtures. Using theory and simulations, we have been able to demonstrate how depletion interactions create oriented “binding” forces between rigid rods to form these “living polymers.” Unlike rod–sphere mixtures in 3D that can demonstrate well-defined equilibrium phases in coexistence, our mixtures

confined to 2D lack these transitions because lower dimensionality favors the formation of linear aggregates, thus suppressing a true phase transition. The qualitative and quantitative agreement between equilibrium and granular patterning for these mixtures suggests that entropy maximization is the determining driving force for bundling. Furthermore, this study un-

covers a previously unknown patterning behavior at both the granular and nanoscales, and may provide insights into the role of crowding at interfaces in molecular assembly.

❖ Jennifer Galanis, Ralph Nossal, and Daniel Harries **Soft Matter** 6:1026–1034 (2010).

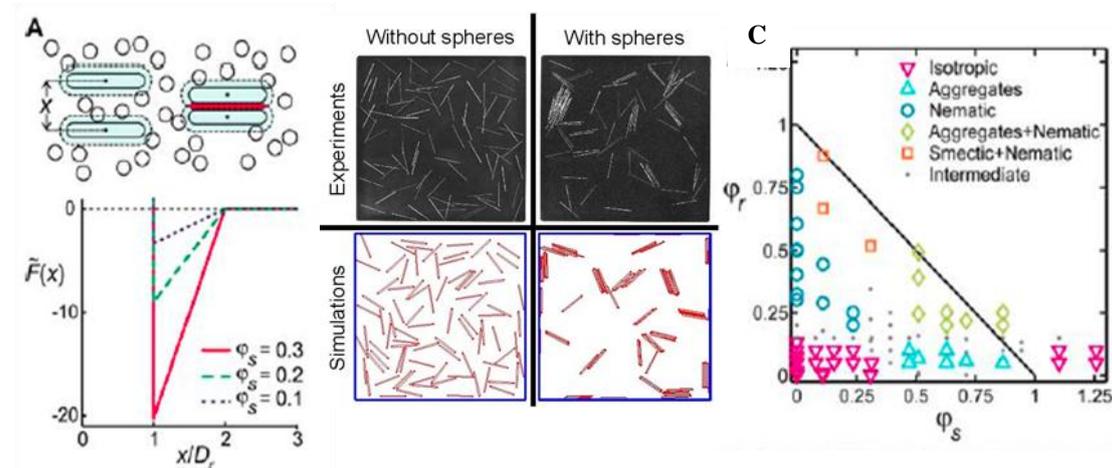


Figure 21: Attractive depletion interactions between hard rods in the presence of sphere crowders favor rod binding and suppress rod slip. Diagrams in A depict the area that rods exclude from spheres (dashed regions) and excluded area overlap (dark shaded regions) when two rods are less than one sphere diameter apart, shown for rod “binding” (A). The free energy gain is greater when there is more overlap that “releases” excluded volume. The experimental realization of this depletion force is seen as clustering of rods when spheres are introduced to rod mixtures (panel B, top, spheres not shown for clarity). The same patterning is achieved in 2D Monte Carlo simulations of hard rods and spheres (Panel B bottom). Panel C shows the wide variety of patterning that is found for different possible combinations of rod and sphere densities.

COLLABORATIONS

- ❖ George Khelashvili, Harel Wienstein (Cornell medical school, NY, NY),
- ❖ Georg Pabst (Austrian Academy of Sciences, Austria), Rachel Yerushalmi-Rozen (BGU)
- ❖ Rudi Podgornik (Slovenia), David Andelman (Tel Aviv U), Dganit Danino (Technion)

CONFERENCE ORGANIZATION SINCE 2006

- ❖ Biophysics mini-symposium (14 Feb 2007, Hebrew University, with Drs. U. Raviv and A. Friedler).

- ❖ From Macromolecular to Cell Biophysics (June 3-4, 2008, Mishkenot, Jerusalem with D. Andelman and W. M. Gelbart).
- ❖ Biomolecular simulations (2009, Safed, with M. Niv, D.T. Major, and K. Levy).

HARRIES GROUP

- ❖ Dr. Jennifer Galanis, Postdoctoral fellow
- ❖ Regina Politi, PhD student
- ❖ Gadiel Saper, Msc Student, 2007-2008: faculty prize for academic achievements
- ❖ Shahar Sukenik, Msc Student (joint with Asaf Friedler)
- ❖ Liel Sapir, BSc student, Dean’s prize 2007, 2008

GRANTS FOR PROFESSOR HARRIES'S GROUP, 2002-2008

Granting Agency	Period	Amount
Israel-Slovenia collaboration, Ministry of Science	2007–2009	\$80,000
Alon Fellowship	2006–2009	\$100,000
Israel Science Foundation (ISF)	2007–2011	\$160,000
Israel Science Foundation (ISF), equipment	2007	\$50,000
Israel Science Foundation (ISF), Workshop	2009	\$17,000
James-Franck Foundation (with Dr. Uri Raviv)	2009	\$100,000

PRIZES, MEMBERSHIPS SINCE 2006

- ❖ Alon Fellowship, 2006
- ❖ Biophysical Society member
- ❖ American Chemical Society member
- ❖ Best teacher award in Faculty of sciences, 2009

RONNIE KOSLOFF

The thrust of my research is quantum molecular dynamics. The interest is in the implication of the underlying basic theory of quantum mechanics on chemical encounters. This is connected to fundamental issues of quantum open systems and quantum thermodynamics.

The field of study this year can be subdivided into:

- ❖ Coherent control
- ❖ Cold Molecules
- ❖ Spectroscopy
- ❖ Quantum Thermodynamics
- ❖ Quantum Methodology

RESEARCH

COHERENT CONTROL

Quantum Control (QC) focuses on guiding quantum systems from initial states to targets governed by time dependent external field. Two interlinked theoretical problem dominate quantum control: controllability and inversion.

Controllability addresses the issue of the conditions on the quantum system which enable control, state-to-state or a more difficult requirement of a unitary transformation in a group of states. In short, a solution to control problem was proved to exist if the combined Hamiltonians of the control and system span a compact Lie algebra. The issue of inversion - of actually finding a control field, is more subtle. Optimal Control Theory (OCT) sets the inversion task as an optimization which is subsequently solved by an iterative approach.

CONTROL BY DECOHERENCE: WEAK FIELD CONTROL OF AN EXCITED STATE OBJECTIVE

Coherent control employing a broad band excitation is applied to a branching reaction in the

excited state. In weak field for an isolated molecule a control objective is only frequency dependent. This means that phase control of the pulse cannot improve the objective beyond the best frequency selection. Once the molecule is put in a dissipative environment a new time scale emerges. We have demonstrated that the dissipation allows achieving coherent control of branching ratios in the excited state.

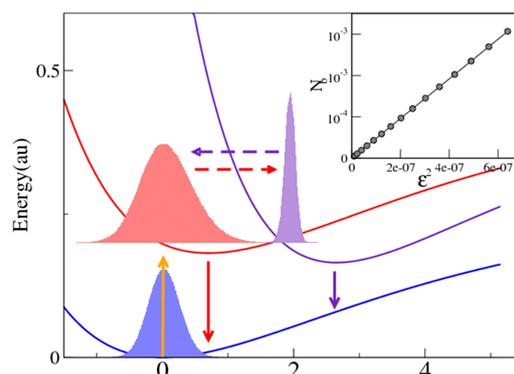


Figure 22: The general scheme: The ground state $\hat{V}_g(r)$, the bright excited state $\hat{V}_b(r)$ and the dark excited state $\hat{V}_d(r)$. Superimposed are snapshots of three wavefunctions: the initial ground state density $\rho_g(r, r)$ the bright state density after the pulse is over $\rho_b(r, r)$ and the dark state density after the transfer $\rho_d(r, r)$ (renormalized). The dotted lines present the absorption and emission from the different final states. The ratio between long time emission of the bright and dark states is an experimental indication of the population ratio between these states. The insert shows the population on the bright state N_b as a function of intensity Ω_0^2 indicating that the calculations within this intensity range are performed in the linear regime.

The model studied contains a nuclear coordinate and three electronic states: the ground and two coupled diabatic excited states (see Figure 22). The influence of the environment is modeled by the stochastic surrogate Hamiltonian. The excitation is generated by a Gaussian pulse where the phase control introduced a chirp to the pulse. For sufficient relaxation we find significant control in weak field depending on the chirp rate. The observed control is rationalized by a timing argument caused by a focused wavepacket. The initial non adiabatic crossing is enhanced by the chirp. This is followed by energy relaxation which stabilizes the

state by having energy lower than the crossing point.

- ❖ G. Katz, M. A. Ratner, and R. Kosloff, "Control by decoherence: weak field control of an excited state objective", *New J. Phys.* **12**, 015003 (2010).

DYNAMIC MATTER-WAVE PULSE SHAPING

We investigated the possibilities for manipulating a matter wave using time-dependent potentials. Assuming a specific setup on an atom chip, we explored how one can focus, accelerate, reflect, and stop an atomic wave packet, with, for example, electric fields from an array of electrodes. We also utilize this method to initiate coherent splitting or an arbitrary wave form. Special emphasis is put on the robustness of the control schemes. We begin with the wave packet of a single atom and extend this to a Bose-Einstein condensate in the Gross-Pitaevskii picture. In analogy to laser pulse shaping with its wide variety of applications, we expect this work to form the base for more complex time-dependent potentials, eventually leading to matter-wave pulse shaping with numerous applications.

- ❖ M. Nest, Y. Japha, R. Folman, and R. Kosloff, "Dynamic matter-wave pulse shaping", *Phys. Rev. A* **81**, 043632 (2010).

COLD MOLECULES

The challenge to achieve a large number of stable ultracold molecules in a trap is the prerequisite for ultracold chemistry. A good starting point is an ensemble of ultracold atoms, where photoassociation has been proven to be an efficient method to form diatomic molecules from a pair of atoms. Those ultracold molecules are in a short-lived electronically excited state: in order to obtain long-lived molecules in the singlet ground or lowest triplet state, a stabilization step has to follow. The initial experiments have used continuous-wave (cw) lasers, and the stabilization of the photoassociated molecule was

achieved by spontaneous emission. As a result the overall process is non-unitary and leads to an ensemble of molecules distributed over many vibrational states. The stabilization step can also be implemented within a two-colour experiment.

PUMP-PROBE SPECTROSCOPY OF TWO-BODY CORRELATIONS IN ULTRACOLD GASES

We developed a scheme for pump-probe spectroscopy to study pair correlations that determine the many-body dynamics in weakly interacting, dilute ultracold gases. A suitably chosen, short laser pulse depletes the pair density locally, creating a "hole" in the electronic ground state. The dynamics of this nonstationary pair density is monitored by a time-delayed probe pulse. The resulting transient signal allows us to spectrally decompose the hole and to map out the pair correlation function.

- ❖ C. P. Koch and R. Kosloff, "Pump-Probe Spectroscopy of Two-Body Correlations in Ultracold Gases", *Phys. Rev. Lett.* **103**, 260401 (2009).

SPECTROSCOPY

We employed wavepacket ideas to simulate ultrafast pump probe spectroscopy in condensed phases and to compare to experiment. A comprehensive study was devoted to the simulation of the photodissociation of CH_3NH_2 .

CHIRP EFFECTS ON IMPULSIVE VIBRATIONAL SPECTROSCOPY: A MULTIMODE PERSPECTIVE

The well-documented propensity of negatively-chirped pulses to enhance resonant impulsive Raman scattering has been rationalized in terms of a one pulse pump-dump sequence which follows the evolution of the excited molecules and dumps them back at highly displaced configurations. The aim of this study was to extend

the understanding of this effect to molecules with many displaced vibrational modes in the presence of condensed surroundings. In particular, to define an optimally chirped pulse, to investigate what exactly it follows and to discover how this depends on the molecule under study. To this end, linear chirp effects on vibrational coherences in poly-atomics are investigated experimentally and theoretically. Chirped pump impulsive probe experiments are reported for Sulforhodamine-B (Kiton Red), Betaine-30 and Oxazine-1 in ethanol solutions with 10 fs resolution. Numerical simulations, including numerous displaced modes and electronic dephasing, are conducted to reproduce experimental results. Through semi-quantitative reproduction of experimental results in all three systems we show that the effect of group velocity dispersion (GVD) on the buildup of ground state wave-packets depends on the pulse spectrum, on the displacements of vibrational modes upon excitation, on the detuning of the excitation pulses from resonance, and on electronic dephasing rates. Akin to scenarios described for frequency-domain resonance Raman, within the small-displacement regime each mode responds to excitation chirp independently and the optimal GVD is mode-specific. Highly-displaced modes entangle the dynamics of excitation in different modes, requiring a multi-dimensional description of the response. Rapid photochemistry and ultrafast electronic dephasing narrow the window of opportunity for coherent manipulations, leading to a reduced and similar optimal chirp for different modes. Finally, non-intuitive coherent aspects of chirp following are predicted in the small-displacement and slow-dephasing regime, which remain to be observed in experiment.

- ❖ A. Wand, S. Kallush, O. Shoshanim, O. Bismuth, R. Kosloff, and S. Ruhman, "Chirp effects on impulsive vibrational spectroscopy: a multimode perspective", *Phys. Chem. Chem. Phys.* **12**, 2149-2163 (2010).

TIME-DEPENDENT QUANTUM WAVE-PACKET DESCRIPTION OF H- AND D-TUNNELING IN N-H AND N-D PHOTODISSOCIATION OF METHYLAMINE AND METHYLAMINE-D₂

The degree to which tunneling through a barrier in the N-H and N-D photodissociation channels of methylAMINE CH_3NH_2 and its deuterated vaRIANT CH_3ND_2 , respectively, plays a role was investigated by time-dependent quantum wave-packet dynamics calculations. Two diMENSIONAL potential energy surfaces PESs of methylamine, presenting the N-H stretch and the HNC bend, were constructed employing multireference ab initio electronic-structure methods, allowing full description of the H motion on the HC - NH₂ plane. The time-dependent SCHRÖDINGER equaTION WAS solved employing the Fourier method for calculating the HamiltonIAN OPERATION TOGETHER WITH THE Chebychev polynomial expansion of the evolution operator. The results show that tunneling and decay to vibrational resonant states on the first excited electronic PES are faster for the H atom than for the D. The decay into two of the resonant states found on the first PES strongly depends on the initially excited vibrational state on the ground electronic.

- ❖ C. Levi, R. Kosloff, Y. Zeiri, and I. Bar, "Time-dependent quantum wave-packet description of H and D atom tunneling in N-H and N-D photodissociation of methylamine and methylamine-d(2)", *J. Chem. Phys.* **131**, 064302 (2009).

QUANTUM TUNNELING OF HYDROGEN ATOM IN DISSOCIATION OF PHOTOEXCITED METHYLAMINE

The probability of hydrogen atom release, following photoexcitation of methylamine, CH_3NH_2 , is found to increase extensively as higher vibrational states on the first excited electronic state are accessed. This behavior is consistent with theoretical calculations, based

on the probability of H atom tunneling through an energy barrier on the excited potential energy surface, implying that N-H bond breaking is dominated by quantum tunneling.

- ❖ R. Marom, C. Levi, T. Weiss, S. Rosenwaks, Y. Zeiri, R. Kosloff, and I. Bar, "Quantum Tunneling of Hydrogen Atom in Dissociation of Photoexcited Methylamine", *J. Phys. Chem. A* **in press** (2010).

QUANTUM THERMODYNAMICS

Quantum thermodynamics is devoted to the study of thermodynamical processes within the context of quantum dynamics. The thermodynamic tradition of learning by example is translated to establishing quantum analogues of heat engines. These studies unravel the intimate connection between the laws of thermodynamics and their quantum origin.

THE QUANTUM REFRIGERATOR: THE QUEST FOR ABSOLUTE ZERO

The emergence of the laws of thermodynamics from the laws of quantum mechanics is an unresolved issue. The generation of the third law of thermodynamics from quantum dynamics is analyzed. The scaling of the optimal cooling power of a reciprocating quantum refrigerator is sought as a function of the cold bath temperature as $T_c \rightarrow 0$. The working medium consists of noninteracting particles in a harmonic potential. Two closed-form solutions of the refrigeration cycle are analyzed, and compared to a numerical optimization scheme, focusing on cooling toward zero temperature. The optimal cycle is characterized by linear relations between the heat extracted from the cold bath, the energy level spacing of the working medium and the temperature. The scaling of the optimal cooling rate is found to be proportional to $T^{3/2}$ giving a dynamical interpretation to the third law of thermodynamics.

- ❖ Y. Rezek, P. Salamon, K. H. Hoffmann, and R. Kosloff, "The quantum refrigerator: The

quest for absolute zero", *Epl* **85**, 30008 (2009).

MAXIMUM WORK IN MINIMUM TIME FROM A CONSERVATIVE QUANTUM SYSTEM

This study considers the problem of obtaining maximum work from a conservative quantum system corresponding to a given change in an external parameter in the Hamiltonian. The example we present is a non-interacting collection of harmonic oscillators with a shared frequency ω which changes from a given initial to a given final value. The example is interesting for its role in experiments at ultra-low temperatures and for probing finite-time versions of the third law of thermodynamics. It is also the simplest system displaying quantum friction, which represents loss mechanisms in any reversible prelude to a thermal process. The example leads to a new type of availability. It is also the first example of a minimum time for transitions between thermal states of a thermodynamic system.

- ❖ P. Salamon, K. H. Hoffmann, Y. Rezek, and R. Kosloff, "Maximum work in minimum time from a conservative quantum system", *Phys. Chem. Chem. Phys.* **11**, 1027-1032 (2009).

MINIMAL TEMPERATURE OF QUANTUM REFRIGERATORS

A first-principle reciprocating quantum refrigerator is investigated to determine the limitations of cooling to absolute zero. If the energy spectrum of the working medium possesses an uncontrollable gap, then there is a minimum achievable temperature above zero. Such a gap, combined with a negligible amount of noise, prevents adiabatic following during the expansion stage which is the necessary condition for reaching $T_c \rightarrow 0$.

- ❖ T. Feldmann and R. Kosloff, "Minimal temperature of quantum refrigerators", *Epl* **89**, 20004 (2010).

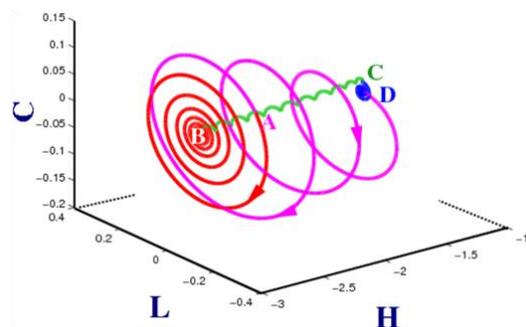


Figure 23: Typical optimal cooling cycle trajectory with linear scheduling shown in the quantum thermodynamical variables energy \hat{H} , Lagrangian \hat{L} and correlation \hat{C} . Point A represents the beginning of the hot *isochore*. Point B represents the beginning of the demagnetization *adiabat*. Point C represents the beginning of the cold *isochore*. Point D represents the beginning of the magnetization *adiabat*. Notice the big difference between the demagnetization and magnetization adiabats.

QUANTUM METHODOLOGY

We renewed our efforts in improving numerical schemes for solving the time dependent Schrödinger equation. The challenge is toward systems with explicit time dependence.

A CHEBYCHEV PROPAGATOR FOR INHOMOGENEOUS SCHRÖDINGER EQUATIONS

A propagation scheme for time-dependent inhomogeneous Schrödinger equations was developed. Such equations occur in time dependent optimal control theory and in reactive scattering. A formal solution based on a polynomial expansion of the inhomogeneous term is derived. It is subjected to an approximation in terms of Chebychev polynomials. Different variants for the inhomogeneous propagator are demonstrated and applied to two examples from optimal control theory. Convergence behavior and numerical efficiency are analyzed.

- ❖ M. Ndong, H. Tal-Ezer, R. Kosloff, and C. P. Koch, "A Chebychev propagator for inho-

ogeneous Schrödinger equations", *J. Chem. Phys.* **130**, 124108 (2009).

A CHEBYCHEV PROPAGATOR WITH ITERATIVE TIME ORDERING FOR EXPLICITLY TIME-DEPENDENT HAMILTONIANS

A propagation method for time-dependent Schrödinger equations with an explicitly time-dependent Hamiltonian is developed where time ordering is achieved iteratively. The explicit time dependence of the time-dependent Schrödinger equation is rewritten as an inhomogeneous term. At each step of the iteration, the resulting inhomogeneous Schrödinger equation is solved with the Chebychev propagation scheme presented. The iteratively time-ordering Chebychev propagator is shown to be robust, efficient, and accurate and compares very favorably with all other available propagation schemes.

- ❖ M. Ndong, H. Tal-Ezer, R. Kosloff, and C. P. Koch, "A Chebychev propagator with iterative time ordering for explicitly time-dependent Hamiltonians", *J. Chem. Phys.* **132**, 064105 (2010).

ALGORITHM FOR SIMULATION OF QUANTUM MANY-BODY DYNAMICS USING DYNAMICAL COARSE-GRAINING

An algorithm for simulation of quantum many-body dynamics having $su(2)$ spectrum-generating algebra is developed. The algorithm is based on the idea of dynamical coarse-graining. The original unitary dynamics of the target observables the elements of the spectrum-generating algebra is simulated by a surrogate open-system dynamics, which can be interpreted as weak measurement of the target observables, performed on the evolving system. The open-system state can be represented by a mixture of pure states, localized in the phase space. The localization reduces the scaling of the computational resources with the Hilbert-

space dimension n by factor $n^{3/2} \ln n$ compared to conventional sparse-matrix methods. The guidelines for the choice of parameters for the simulation are presented and the scaling of the computational resources with the Hilbert-space dimension of the system is estimated. The algorithm is applied to the simulation of the dynamics of systems of 2×10^4 and 2×10^6 cold atoms in a double-well trap, described by the two-site Bose-Hubbard model.

- ❖ M. Khasin and R. Kosloff, "Algorithm for simulation of quantum many-body dynamics using dynamical coarse-graining", Phys. Rev. A **81**, 043635 (2010).

DELETERIOUS EFFECTS OF LONG-RANGE SELF-REPULSION ON THE DENSITY FUNCTIONAL DESCRIPTION OF O₂ STICKING ON ALUMINUM

Density functional theory (DFT) with semilocal functionals such as the local-density and generalized gradients approximations predicts that the dissociative adsorption of oxygen on Al (111) goes through without a barrier in stark contradiction to experimental findings. This problem motivated our study of the reaction of oxygen colliding with a small aluminum cluster Al₅. We found semilocal functionals predict a minute barrier to sticking, associated with smeared long-range charge transfer from the metal to the oxygen. Hybrid B3LYP predicts a

larger barrier while the range-separated the Baer-Neuhauser-Livshits (BNL, Phys. Chem. Chem. Phys. 2007, 9, 2932.) functional finds a more prominent barrier. BNL predicts short-ranged and more abrupt charge transfer from the surface to the oxygen. We conclude that spurious self-repulsion inherent in semilocal functionals causes early electron-transfer, long-range attraction toward the surface and low reaction barriers for these systems. The results indicate that the missing DFT barrier for O₂ sticking on Al (111) may be due to spurious self-repulsion.

- ❖ E. Livshits, R. Baer, and R. Kosloff, "Deleterious Effects of Long-Range Self-Repulsion on the Density Functional Description of O₂ Sticking on Aluminum", J. Phys. Chem. A **113**, 7521-7527 (2009).

OVERVIEW

Our efforts in coherent control was divided between the issues of controllability, optimal control theory (OCT) and application ultracold matter. In quantum thermodynamics we concentrated on discrete four stroke models of quantum refrigerators and their optimal performance. In particular the approach to the absolute zero. The practical challenges led to the development of new propagation algorithms.

ACTIVE GRANTS FOR PROFESSOR KOSLOFF

Granting Agency	Period	Amount
Niedersachsen	07.2010 – 08.2007	€ 112,500
D.F.G	12.2009 – 07.2007	€ 116,900
Homeland security	06.2009 – 07.2008	\$ 31,000
Quantum Computing	11.2009 – 11.2008	\$ 25,500
Government Grant	12.2009 – 11.2005	≈ 115,000
ISF	09.2009 – 10.2007	≈ 334,000
Government Grant	10.2009 – 08.2007	≈ 400,000

GERMAN COLLABORATIONS

Name	Affiliation	Field
Prof. Dr. Cederbaum. L.	University of Heidelberg	Quantum Many Body Dynamics
Prof. Dr. Freund, H.-J.	FH, MPG, Berlin	Photodissociation on Surfaces

Prof. Dr. Hasselbrink, E.	Univ. of Duisburg- Essen	Oxygen Dissociation on Surfaces
Prof. Dr. Hoffmann, K.-H.	University of Chemnitz	Quantum Thermodynamics
Prof. Dr. Klüner, Th.	Theoretical Chemistry, University of Oldenburg	Coherent Control and Surface Reactions
Dr. Koch, Ch.	FU Berlin	Coherent Control / Cold Molecules
Dr. Nest. M.	TU, Munich	Many Body Quantum Mechanics
Dr. Poschinger, U.	University of Freiburg	Cold Molecules
Prof. Dr. Tieman, A.	University of Hannover	Cold Molecules
Prof. Dr. Weidenmüller, H.-A.	University of Heidelberg	Cold Molecules
Prof. Dr. Wester, R.	University of Freiburg	Cold Molecules
Prof. Dr. Wöste, L.	FU Berlin	Coherent Control / Cold Molecules

RAPHAEL D. LEVINE

NEW DIRECTIONS IN THE STRUCTURE, ENERGETICS AND DYNAMICS OF COMPUTING BY MOLECULES

With the cooperating German investigators:

- ❖ Karl L. Kompa, Max-Planck-Institut für Quantenoptik, Garching
- ❖ Rainer Weinkauff, Heinrich-Heine-Universität Duesseldorf.
- ❖ Rainer M. Waser and Sylvia Karthäuser, Forschungszentrum Juelich
- ❖ Thomas Halfmann, TU-Darmstadt

And with the cooperation of

- ❖ Françoise Remacle, Université de Liège, Liège, Belgium

We report on a direction of research that we did not highlight in reports of previous years. We discuss Non-Boolean logic and parallel computation on a realistic ladder of molecular energy states and the design and implementation of combinational and finite state machines. The large volume of work requires that we concentrate on one topic and we chose the characterization with *ab initio* and quantum dynamical studies the energetic, structural and dynamical molecular properties relevant for implementing combinational circuits on a pair of atoms. Not reviewed is our progress in ternary logic as published in Applied Physics Letters and in Nature Nanotechnology, our work on parallel computing

published in the festschrift in honor of Jorn Manz and the work on computing via molecular recognition published in Nature Nanotechnology.

IMPLEMENTATION OF A CYCLABLE FULL ADDER BY ELECTRICAL ADDRESSING OF A DONOR MOLECULE IN SILICON.

This work is submitted (but not yet accepted) to the festschrift in honor of Mark Ratner.[7]

The physical system we consider is a single electron bound to a shallow-donor pair (e.g., P_2^+) in silicon, subject to a time-dependent electric field that controls the localization of the charge on one or the other dopant atom. In principle, the electric field can be applied parallel or perpendicular to the Si-SiO₂ (001) interface. We discuss here the case where the electric field is applied parallel to the interface, using a source and a drain electrode. Figure 1 shows a schematic of the structure. We also investigated the case where the field is applied perpendicular to the interface.

The geometry of the device that we consider here is different from previous proposals²⁻⁵ because the two donors are not placed at equal distance from the interface. (In figure 1, $R_1 \neq R_2$). Since the ionization potential of the dopant atom is controlled by its distance to the interface (see figure 2), this gives us the ability to build a 'heteronuclear' dopant molecule, and in principle to control the degree of covalent vs. ionic bonding, using dopant atoms of the same chemical na-

ture, here phosphorous. This flexibility is important for the design of logic schemes.

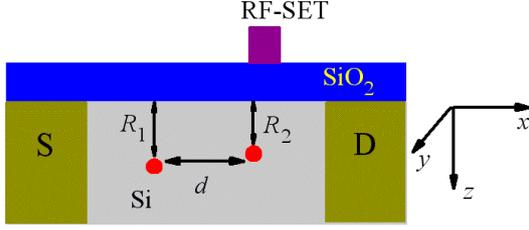


Figure 24: Schematic of the structure: two donor atoms are placed at the depths R_1 and R_2 (along the z direction) from the Si-SiO₂ interface and separated by a distance $d = |x_1 - x_2|$ in the x direction. The two electrodes, marked S and D, are used to apply an electric field along the x direction. The RF-SET used to detect the charge on the right dopant atom is also shown.

The conduction band of silicon has six equivalent minima located near the X-points of the Brillouin zone. Symmetry breaking at the site of the dopant atom leads to valley-orbit (VO) coupling and lifts the degeneracy of the ground state that is predicted by the single-valley formulation of effective mass theory.[8] More refined treatments that include the valley-orbit coupling have been proposed at the effective mass theory level⁷⁻¹⁰ and beyond it, at the tight-binding¹¹⁻¹⁵ and atomic computational levels.[9] As shown below, the field strengths required for charge switching between the two weakly coupled donors are ≈ 0.01 kV/cm when the field is applied parallel to the interface (see fig. 3) and 0.5 kV/cm when it is applied perpendicular to it (not shown). These field strengths will therefore not induce coupling between the GS of the dopants and the higher energy states of the manifold arising when the VO coupling is taken into account. In our logic implementation, only the two GS of the pair of dopant atoms are coupled and they are well separated in energy for the other states. For this reason, we use the single-valley approximation since it allows us to capture the essential physical aspects of the formation of the two lowest energy states of the molecular ion, made from the linear combination of the GS states of the two dopants. These are the electronic states used to implement the logic scheme for a full addition. However, we plan to take advantage of the manifold of states induced by symmetry

breaking at the donor site for the implementation of parallel logic schemes by electric addressing.

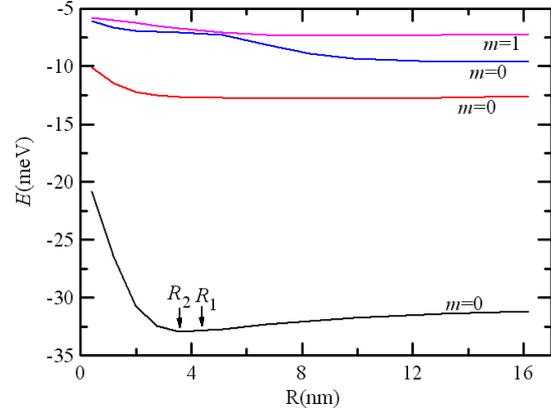


Figure 25: Energies of the 5 lowest states of a shallow donor impurity near the (001) surface of Si as a function of the distance, R , to the interface. The states are labeled by the value of the magnetic quantum number, m . The arrow indicates two values, $R_1 = 4.3$ nm and $R_2 = 3.6$ nm, see figure 1, that were used in the results reported below for the two-donor case.

In the single-valley approximation the time-dependent Hamiltonian for N dopants written in cartesian coordinates reads

$$\begin{aligned}
 H(t) = & - \left[\frac{\hbar^2}{2m_{\perp}} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{\hbar^2}{2m_{\parallel}} \frac{\partial^2}{\partial z^2} \right] \\
 & - \sum_{i=1}^N \frac{e^2}{\epsilon_{\text{Si}} \sqrt{(x-x_i)^2 + y^2 + (z-z_i)^2}} \\
 & + \sum_{i=1}^N \frac{Qe^2}{\epsilon_{\text{Si}} \sqrt{(x-x_i)^2 + y^2 + (z-z_i)^2}} \\
 & - \frac{Qe^2}{4\epsilon_{\text{Si}}z} + e\mathbf{F}(t) \cdot \mathbf{r}
 \end{aligned} \tag{6}$$

where the first term is the kinetic energy of the electron, the second is the time-dependent external electric-field potential, the third is the Coulomb potential of the two centers and the fourth and the last are the image-charge potential of the donors and of the electron. $m_{\perp} = 0.191m_e$ and $m_{\parallel} = 0.916m_e$ (m_e is the mass of a free electron) are the transverse and longitudinal effective masses, respectively, and N is the number of donors. In the logic device that we discuss below, there are $N = 2$ dopants.

$Q = (\epsilon_{\text{SiO}_2} - \epsilon_{\text{Si}}) / (\epsilon_{\text{SiO}_2} + \epsilon_{\text{Si}})$ where $\epsilon_{\text{Si}} = 11.4$ and $\epsilon_{\text{SiO}_2} = 3.8$. [10, 11] The ground state and lowest excited state wave functions at zero and finite fields are solved for numerically on a grid by the Lanczos method. [12]

We first consider a single donor ($N = 1$) in the absence of an electric field. The results will serve as a basis for discussing the two-center ($N = 2$) case. The donor is located at a distance R from the interface and figure 2 shows the five lowest eigenenergies as a function of R . Our results are consistent with those of ref. [10], where the energies were obtained by a variational method. For the one dopant case, the system is cylindrically symmetric and therefore the magnetic number m is a good quantum number. In figure 2, the three lowest states (from bottom to upper) labeled by $m=0$ corresponds to the $1s$, $2p_z$, and $2s$ orbitals of a hydrogen atom, and the states labeled by $m=1$ are doubly degenerate, corresponding to the $2p_x$ and $2p_y$ orbitals.

By positioning the two dopants at a slightly different distance from the interface and far from each other so that they are weakly coupled, it is possible to almost completely localize the electron on the left or on the right in the ground state of the two-donor molecule, without applying any external field. In the configuration shown in figure 1, the left dopant is placed at $R_1 = 4.3$ nm from the interface, the right dopant at $R_2 = 3.6$ nm and the two dopants are separated by 32 nm. In this configuration the right dopant has a lower energy than for the left dopant (see figure 2) and since the two dopants are very weakly coupled, in the ground state of the dopant molecule, the electron is localized on the right dopant atom (positive x coordinate). The hole is then on the dopant on the left. We denote the ground state of the one electron two dopant molecule as L^+R . The opposite is the case for the first excited state that is denoted LR^+ .

The electron charge distribution can be shifted by applying a static electric field. In a strong field is applied along the x direction, $F_x = 0.01$ kV/cm, the ground state is of the form LR^+ with the elec-

tron localized on the left dopant and in the excited state, L^+R , the electron is localized on the right.

The reversal of the polarity of the charge orientation with the field applied in the x direction is shown vs. the field strength in figure 3. In figure 3a, the energies of the ground and first excited states are plotted as a function of F_x (in kV/cm) while the gap between the two states is shown in panel b. The maximum energy gap, $\Delta_0 = 0.016$ meV, occurs at 0 and 0.01 kV/cm field strengths and is governed mainly by the position of the two donors with respect to the interface (see figure 1). The minimum gap, $\Delta_{\text{min}} \approx 0.0024$ meV occurs when the two levels anti cross, for $F_x = 0.005$ kV/cm. This value is determined primarily by the lateral distance d between the two centers. The two energy gaps set the time limits of the proposed operation for the logic machine. In particular, the minimum gap, Δ_{min} , determines how fast a diabatic transition (meaning a curve crossing in panel a of figure 3, E.g., L^+R to L^+R) must be for a diabatic state to be maintained as the field is changing. In order to ensure a clear difference between the adiabatic and the diabatic charge transfer, the value of the maximum energy gap Δ_0 must be large compare to Δ_{min} .

An adiabatic transition means that the quantum state is maintained and so the field change needs to be done slowly, and slower than $\hbar/\Delta_{\text{min}}$. A diabatic transition requires that the field is swept across the gap between the two adiabatic states in a time shorter than $\hbar/\Delta_{\text{min}}$ see e.g., [13]. The faster the diabatic switching, the better the localization of the electron on a given site is preserved. Since we cannot currently switch an electric field in much less than 100 ps, at best the following of a diabatic path requires a minimal gap, Δ_{min} , much smaller than 0.04 meV.

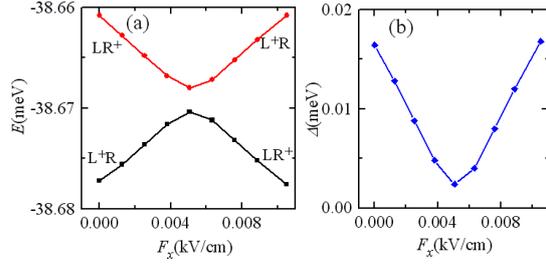


Figure 26: (a) The ground state and the first excited energies of a single electron bound to a shallow-donor pair as a function of the electric field strength (in kV/cm) applied in the x direction. Here L+R means that the wave function of the electron is localized at the right donor while LR+ means that the wave function is localized at the left donor. (b) Gap between the two states, Δ (meV), as a function of the field strength.

The full addition is implemented as a non linear finite state machine, using a pulse voltage with an asymmetric time profile :

$$F_x(t) = \begin{cases} F_{\max} \exp\left(-\frac{(t-t_{on})^2}{2t_w^2}\right) & t \leq t_{on} \\ F_{\max} & t_{on} < t \leq t_{off} \\ F_{\max} \exp\left(-\frac{(t-t_{off})^2}{2t_w'^2}\right) & t > t_{off} \end{cases} \quad (7)$$

where $t_w = 10$ ns is the adiabatic switching constant, and $t_w' = 100$ ps the diabatic switching off constant, (see equation (7)). These switching times ensure that the switching-on process ($t < t_{on}$) of the electric field is long so that it is an adiabatic process where the quantum state of the system is maintained as can be seen in figure 4. Say that the system is initially and in the absence of the field in the ground state, cf. figure. 4a. Then the electron is localized around the right donor. By adiabatically switching on the electric field we move the electron from the right donor to the left, or from state L+R to LR+. In such a process the system stays in the ground state meaning that its energy follows the lower curve in figure 3. The quantum state is preserved even though the electron has switched sides. Next, at t_{off} , we suddenly switch off the field very fast. The system has little time to adjust to this change and continues to stay at essentially the same state of the electron, namely LR+. Since this state is not an exact eigenstate of the Hamil-

tonian at the final stage (when $F_x = 0$), the charge density oscillates with a small amplitude around a mean value that is not exactly 1 or 0.

The net effect after one cycle, duration 40 ns in figure 4, is that the electron is moved from a zero field state L+R to a zero field excited state LR+, going through the intermediate state LR+ at finite field. This intermediate state is actually the ground state of the system when the field is on. In figure 4b, we show the complementary situation, where the initial state at zero field is the excited state of the donor pair, localized on the left donor.

The full adder operates as a finite state machine. We use four internal states of the machine: two levels at zero field and two at a finite gate field. The two levels at zero gate are the ground state L+R (electron localized on the right) and the first excited state LR+(electron on the left) while at finite high field the ground state is LR+(electron on the left) and the first excited state is L+R (electron localized on the right), see figure 3.

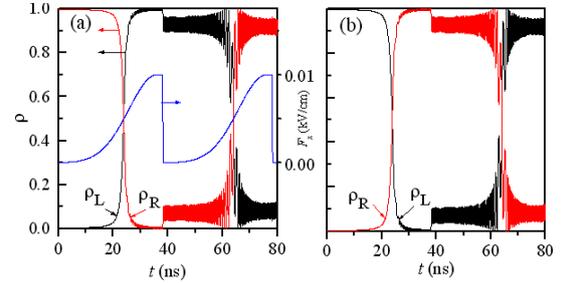


Figure 27: Computed charge densities on the left and on the right dopants, ρ_L and ρ_R , as a sequence of two pulses is applied to the two donor pair. The total duration of one pulse is 40 ns. The shape of the pulse is given by equation (7) and its time dependent strength is shown on the left ordinate axis of panel (a) (blue). $t_{on} = 36$ ns, $t_{off} = 38$ ns, $t_w = 10$ ns, and $t_w' = 100$ ps. $F_{\max} = 0.01$ kV/cm. In (a), the initial condition is the ground state when $F_x = 0$. In (b), the initial condition is the first excited state when $F_x = 0$.

A full addition is a logic operation with three inputs, a ‘carry in’ digit that comes from the previous addition and two input digits that need to be added. The addition has two outputs, a ‘sum out’ that is the digit representing addition modulo 2 of the two input digits and the ‘carry out’ that becomes the ‘carry in’ for the next addition.

We store the ‘carry in’ bit in an internal state of the machine at zero field. We take that the electron on the right, that is L^+R , corresponds to the logic value 0, while the electron on the left, that is LR^+ , corresponds to the logic value 1. For the machine to be cyclable it is necessary that at the end of the addition the ‘carry out’ digit is stored as an internal state of the machine, ready to be used as the ‘carry in’ bit for the next addition.

The first digit to be added is encoded in applying or not a voltage pulse. If the digit to be added has logical value 0, no pulse is applied while if the digit has the value 1, a pulse is applied.

The localization of the electron is changed from left to right or vice versa when the pulse field is applied, which performs a XOR (or addition modulo 2) operation between the input and the state of the machine. The intermediate carry

output is encoded into the localization of the electron on the right dopant at high field, before it is diabatically switched off. If the electron is localized on the right dopant at high field, the intermediate carry has logical value 1 and if not, it has logical value 0. The measure of the charge of the right dopant at high field corresponds to the AND operation between the input digit and the state of the machine and gives the intermediate carry.

The full addition proceeds in two cycles. During the first cycle, the device performs the half addition of the ‘carry in’ digit which is already in its memory and one of the inputs. This intermediate cycle leads to an ‘intermediate carry out’ and an ‘intermediate sum’. The operations are summarized in the traditional form for logic namely a ‘transition table’, in Table 3.

Table 3: Operation of the first half adder that realizes that addition of the ‘carry in’ and one of the input digits. The initial state, left column, is the state of the machine that stores the ‘carry in’. The value of the ‘carry in’ is shown as the argument. The voltage is not or is applied depending on the value of the bit, 0 or 1, to be added. (The state of the machine is read at the end of the pulse when the field is zero). The eXclusive OR (or XOR) operation is the intermediate sum. The charge on the left or on the right dopant as given in the last two columns is measured at the plateau of the field strength where the field is maximal. For a half addition it is sufficient to read the charge on the dopant on the right. The table also shows that the measure of the charge on the left dopant at high field corresponds to an inhibit, INH, operation, which enables to implement a half subtraction in parallel with the half addition.

Initial state	Voltage pulse	Intermediate state = intermediate sum = output of XOR	Output of AND operation (C_1) = Charge on right dopant R at F_{max}	Output of INHhibit = Charge on Left dopant at F_{max}
L^+R (0)	0	L^+R (0)	0	0
L^+R (0)	1	LR^+ (1)	0	1
LR^+ (1)	0	LR^+ (1)	0	0
LR^+ (1)	1	L^+R (0)	1	0

At the end of the first half addition, the intermediate sum is stored as the state of the machine and the first carry output, C_1 , has been measured at the high field end. In the second half addition, Table 4, the second input digit is added to the intermediate sum, leading to the sum out and the second carry C_2 . The sum out is the state of the machine at zero field, after the second pulse is over. The C_2 output is given by the value, 0 or 1, of the charge on the right dopant at high field. Since the two carries, C_1 and C_2 , cannot be 1 simultaneously, to detect a charge on the right dopant at high field during either one of the two cycles means that the carry out is 1.

The full adder logic scheme discussed above can be experimentally realized by integrating the two donor system with a single electron transistor (RF-SET) and a pulse gate. It has been shown that this experimental set-up allows for fast electrical read-out and control of the double donor charge state.[14] SETs operating at radio frequencies (RF-SETs) are proven to be fast and highly sensitive charge detectors, allowing electrometry with subelectron resolution down to the quantum limit[15]. Charge sensitivities of $10 \mu e/Hz^{1/2}$ at megahertz bandwidth were demonstrated using silicon RF-SETs[16]. The entire gate pulse sequence for a full adder requires three pulses,

which rise adiabatically and fall suddenly. The first pulse sets the system in its initial state, depending on the carry-in. The next two pulses correspond to the logic inputs and are kept at F_{max} for a time long enough ($\sim \mu s$) for the RF-SET to measure whether the charge is on the right

dopant. After applying these pulses the final state of the system, that is the sum, is read out by the RF-SET. The total length of a pulse sequence is much shorter than the computed decoherence lifetime of the system,[14, 17] which was experimentally verified in ref. 9

Table 4: Operation of the second half adder that realizes that addition of the intermediate sum and the second of the input digits. The state of the machine is always defined at zero field. The charge on the left and right dopant is measured at the maximum field strength.

Intermediate state = intermediate sum	Voltage pulse	Final State = Sum out	Charge on R at F_{max} = output of AND (C_2)	Charge on L at F_{max} = output of INH
$L^+R(0)$	0	$L^+R(0)$	0	0
$L^+R(0)$	1	$LR^+(1)$	0	1
$LR^+(1)$	0	$LR^+(1)$	0	0
$LR^+(1)$	1	$L^+R(0)$	1	0

To reset the system to the ground state, the electron is first drained to a nearby decoupled reservoir by applying a field pulse. Then an electron is loaded to the right dopant by increasing the coupling between the reservoir and the double donor system. This reset procedure will return the system to the ground state of the donor pair at zero field, whether the final state was the ground or the excited state.

To summarize, we showed that it is possible to implement a full adder by controlling electron localization with voltage pulses in the two lowest excited states of a donor pair molecule. Time-dependent simulations based on the effective mass model for the donor molecule support the proposed logic scheme, that can be realized on a CMOS compatible device, using realistic switching and acquisition times and a RF-SET for charge detection.

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PROFESSOR LEVINE'S GROUP 2002-2008

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Dr. Menashe Rajuan,	PhD	Hi-Tech company
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Noa Richke	MSc	Politics

MASHA Y. NIV

Since its establishment in 2007 at the Faculty of Agriculture, Food and Environment at HUJI, my lab has been focusing on molecular recognition and conformational dynamics in two major signal transduction families - protein kinases and G-protein coupled receptors (GPCRs). We pursue specific questions in collaboration with experimental labs and develop new generally applicable computational approaches inspired by these biological questions.

PROTEIN KINASES

Protein kinases play a crucial role in cell regulation, have many links to diseases, and therefore are major therapeutic targets. These highly dynamic proteins often participate in large complexes, and exhibit multiple regulation strategies. All kinases bind adenosine triphosphate (ATP), but each kinase has its own set of substrate proteins. We are therefore focusing on inhibition of

kinase-substrate and other kinase-protein interactions, with the goal to obtain highly specific inhibitors.

BINDING POCKETS ANALYSIS

One of the novel approaches to inhibition of protein-protein interactions is by utilizing peptides, peptidomimetics and other large and flexible molecules. Due to their flexibility and large number of degrees of freedom compared to the conventional "drug-like" molecules, novel computational methods need to be developed to address the challenge of rational design of such molecules [1]. To unravel the basis of specificity of kinase recognition of their substrates, we are analyzing the binding pockets of human protein kinases.

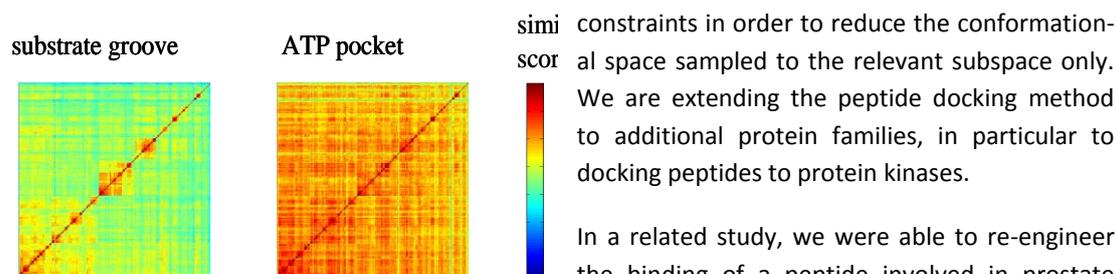


Figure 28: Substrate binding site is more variable than ATP binding site - Similarity scores between substrate binding grooves and between ATP pockets in all pairs of Ser/Thr kinases. ATP pockets are almost identical, in contrast to the more variable substrate binding groove. (From Rubinstein and Niv, poster presented at Israeli Bioinformatics Symposium April 2009)

We constructed sub-alignments, containing only the pocket residues for each substrate position, and used them to calculate similarity scores for each pair of kinases. Our main results, presented at the Israeli Bioinformatics Symposium, April 2009 are:

Both the phosphoacceptor-binding and the preceding residue pockets can differentiate between the Ser/Thr and the Tyr kinases, and are highly conserved within each super-family. The rest of the substrate binding groove is hyper-variable, in contrast to the highly conserved ATP-binding pocket. We are continuing to explore the substrate binding groove of kinases with the goal of rational design and refinement of peptidomimetic and peptidic inhibitors of kinases, a direction we have been pursuing in the recent years [2-4].

PEPTIDE DOCKING

The prediction of the structure of a complex between a protein and a peptide ("peptide docking") is a crucial step towards the ability to rationally design peptides for regulation of signal transduction. This task is a daunting one, due to the highly flexible nature of the peptides. We have developed a Simulated Annealing Molecular Dynamics algorithm for peptide docking [5]. An important feature of our algorithm, which was subsequently embraced by other peptide docking methods, is to include knowledge-based

constraints in order to reduce the conformational space sampled to the relevant subspace only. We are extending the peptide docking method to additional protein families, in particular to docking peptides to protein kinases.

In a related study, we were able to re-engineer the binding of a peptide involved in prostate cancer relevant signaling pathway [6]: Neutral endopeptidase (NEP) is a cell-surface peptidase that is normally expressed by numerous tissues but whose expression is lost or reduced in a variety of malignancies. Using experimental data, threading, and sequence analysis, we predicted the region involved in binding to the NEP cytosolic domain in a partner protein. In collaboration with David Nanus lab, we were able to both design interaction-disrupting mutations and to engineer a related non-binding protein into a NEP-binder [6].

PROTEIN DYNAMICS

Because physiologically relevant motions of proteins are too slow to be accessed by atomistic molecular dynamics simulations, we are aiming at ways of coarse-graining the protein structures. The idea is to identify subregions in proteins that move as semi-rigid blocks (or "beads") and to reduce the number of interactions and forces that need to be calculated during the dynamics simulation, making the simulation more efficient. One elegant approach to achieve this goal was proposed by Essiz and Coalson [7]. Several methods exist for the identification of protein domains (i.e. independently folding units) and motion hinges. Fewer methods are aimed at identifying rigid substructures or sub-regions within a domain. Most of them depend on comparison between two input structures or partition the structure only to rigid blocks, without considering possible flexible regions, e.g. loops and linkers.

BlockMaster [8] is a new method we are developing for partitioning protein structures into semi-rigid blocks and flexible regions. The method is based on residue-residue correlations

calculated from normal modes of a single input structure. According to our hypothesis, structural regions that remain semi-rigid during the functional dynamics of a protein are comprised of residues that have highly correlated motion in the lowest-frequency normal modes. Thus, our criterion for inclusion of a residue into a rigid block was high motional correlation with the rest of the residues in the same block. Correlation C_{ij} between residues i and j was calculated as the average correlation summed over 100 lowest frequency non-trivial normal modes, shown to be enough for convergence.

$$C_{ij} = \frac{\sum_{l=7}^{106} \frac{U_{il} U_{jl}}{\Omega_l}}{\left(\sum_{m=7}^{106} \frac{U_{im} U_{im}}{\Omega_m} \right)^{\frac{1}{2}} \left(\sum_{n=7}^{106} \frac{U_{jn} U_{jn}}{\Omega_n} \right)^{\frac{1}{2}}}$$

Blocks were identified using correlation matrix and distance matrix. Each block was started from two currently most correlated atoms. The rest of the atoms, which are not yet assigned to a blocks, were checked. Atom most correlated and nearest to the atoms which are already assigned to the block, was chosen to be added to this block. To validate the method, we showed that BlockMaster partitions protein structures are in agreement with expert opinion using a test set of five two-domain proteins and on single-domain proteins which had been divided into subdomains by experts: GroEL, adenylate kinase (ADK) and citrate synthase [8], Figure 29.

BlockMaster division of protein kinases into semi-rigid blocks was next analyzed. The distribution of the aliphatic residues between blocks (Table 5) is in agreement with the expectation that the semi-rigid regions would correspond to the hydrophobic core, while the flexible regions would have residues that ensure conformational flexibility and less secondary structure. Notably, our results were obtained without explicitly representing the physicochemical properties of the residues or hydrophobic, electrostatic, and other terms of the potential since a simplified Hookean potential was used for all residues. The

fact that the partition of the residues into the flexible and the rigid subgroups agrees with their properties stems from the fact that the residue's character dictates the folded structure, and this structure, in turn, determines the dynamics.

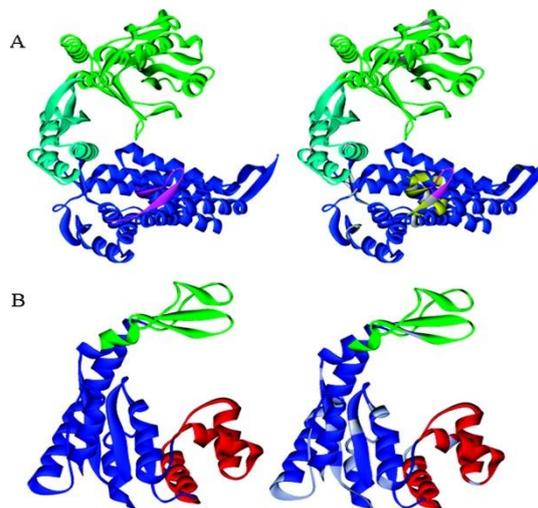
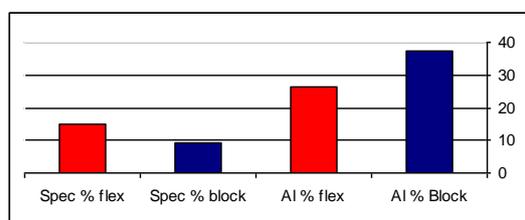


Figure 29: Illustration of BlockMaster performance for well established testcases - A) GroEL: left panel, the accepted partition into subdomains (represented by different colors) in the literature; right panel, partitioning by BlockMaster. B) adenylate kinase: left panel the accepted partition in the literature; right panel, partitionin by BlockMaster, from ref. 8)

The protein kinase structure is traditionally divided into an N-lobe and a C-lobe. A change in inter-lobe orientation is an important hallmark of activation. The lobes themselves are far from being rigid since the orientation of the α C helix within the N-lobe and that of the activation loop in the C-lobe are key aspects of kinase activation. Many of the flexible residues were the same for the different (Ser/Thr and Tyr, active and inactive) protein kinase structures that we analyzed. The main conclusions from these results are that the C-lobe has more consensus rigid blocks than the N-lobe; and that the main difference between the S/T kinases and Tyr kinases is the higher flexibility of the Tyr kinases in the substrate-binding regions. These regions were described in detail in our previous work and used as the basis for deriving kinase-specific inhibitory peptides[2-4]. The connection between flexibility and substrate recognition will be explored in future work. Some differences were apparent

between blocks calculated in the inactive structures and those in the active structures. Therefore, "freezing" of blocks identified in one of the conformations could prevent undergoing the conformational change needed to achieve the other conformation. A possible solution to this problem could be "on-the-fly" application of the BlockMaster procedure to intermediate snapshots along the trajectory. To this end, full atomistic MD simulations of Protein Kinase B were carried out (Cheng and Niv, submitted) and application of BlockMaster to PKB and other long trajectories is underway.

Table 5: Difference in physicochemical composition of residues in flexible vs. block regions in protein kinases. Spec – Special conformation (Gly, Pro). Al – Aliphatic residues (from supplementary data of ref. 8)



G-PROTEIN COUPLED RECEPTORS

GPCR OLIGOMERIZATION

G-protein coupled receptors (GPCRs) play a key role in multiple physiological processes and are involved also in taste and odor sensing and many medical conditions, including metabolic disorders. For many GPCRs dimerization was established in cells, but the functional role of dimerization is not always clear. We are aiming to delineate this role by designing dimerization interface-disrupting mutants. We have modeled the monomer structure of a serotonin receptor and used several approaches (including protein-protein docking) to suggest a dimeric interface of these monomers. The interface was analyzed to suggest disrupting mutations. The mutants are tested in the lab of Prof. Ponimaskin from the Hannover Medical School, Germany (Niedersachsen-Israel Research cooperation funded project). The experimental results for mutant dimerization support our computationally predicted in-

terface (manuscript in preparation). Prof. Ponimaskin visited our lab in March 2009 and May 2010 and a reciprocal visit is planned for August 2010.

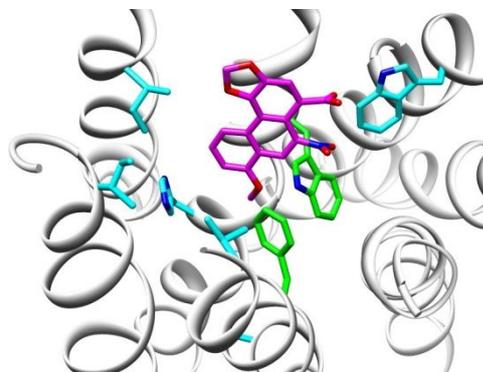


Figure 30: A model of interaction between the bitter aristolochic acid and bitter taste receptor hTAS2R14. Residue for which involvement in ligand binding was confirmed experimentally are shown in green. (Levit, Deutschmann, Behrens, Meyerhof and Niv, unpublished)

HOMOLOGY MODEL-ASSISTED BINDING SITE PREDICTION

While typically an endogenous ligand activates its cognate receptor in a highly specific manner, the receptors for bitter taste recognize and are activated by a large array of seemingly dissimilar compounds found in food. We aim to delineate the specificity of interactions between taste receptors and their ligands, and to be able to predict bitterness of compounds. This project is a collaboration with Prof. Meyerhof and Dr. Behrens at DIFE (German Inst Human Nutr in Potsdam Rehbrucke, Germany). The homology modeling, sequence and structure-based analysis and ligand-docking approaches in our lab is combined with site-directed mutagenesis and functional assays in the DIFE lab to identify binding modes of bitter tastants [9].

A pre-proposal to DFG with Prof. Wolfgang Meyerhof and Dr. Maik Behrens (The German Institute of Human Nutrition Potsdam-Rehbruecke) and Dr. Rafik Karaman and Dr. Hatem Hejaz (Pharmacy College, Al-Quds University, Jerusalem) has been approved and a full proposal is to be submitted in the next weeks. Visits to DIFE took place in August 2008 and Feb-

bruary 2010, with an additional visit planned for August 2010.

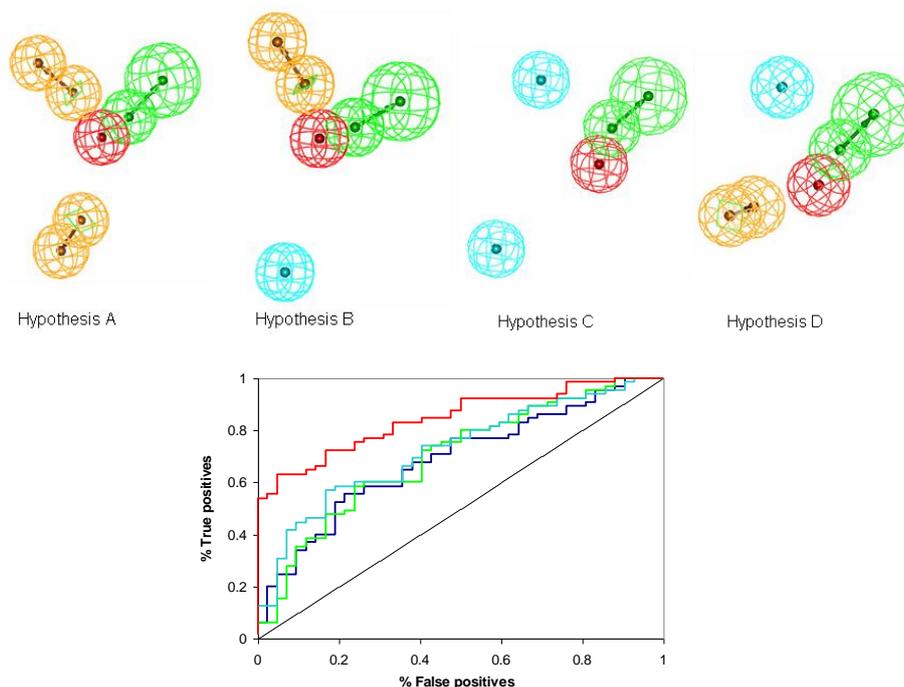


Figure 31: Four feature pharmacophore can discriminate between known active and inactive PKR antagonists. (Top) The pharmacophores are represented as tolerance spheres with directional vectors where applicable. Green spheres represent hydrogen bond donors, red - positive ionizable, light blue - hydrophobic and orange - aromatic ring. (Bottom) ROC curves obtained for the four hypothesis, showing capability of each hypothesis to distinguish between active and inactive molecules. Blue line - A, green - B, light blue - C, red - D, black - by random selection

LIGAND CHARACTERIZATION

In ligand-based practices of drug design, molecules are evaluated by their similarity to a characteristic fingerprint of known ligands. Anat Levit, a PHD student in the lab, used a dataset of 68 known antagonists of a novel GPCR, the Prokineticin Receptor (PKR). Three compounds presenting the highest biological activity ($IC_{50} < 0.02\mu M$) were used as templates for common feature pharmacophore generations, using the HipHop algorithm [10], which identifies common 3D spatial arrangements of chemical features in a given dataset. Four pharmacophore hypotheses were generated (A-D), each with four chemical features. As seen in Figure 31(top), all hypotheses share a hydrogen acceptor and positive ionizable features, and vary in degree of hydrophobicity tolerated: hypothesis A is the most restrictive, presenting two aromatic ring features, while hypothesis C is the most promi-

cuous, presenting two general hydrophobic features. To assess the validity of these hypotheses in differentiating between known biologically active and inactive compounds, receiver operating characteristic (ROC) curves for each hypothesis were generated (Figure 31(bottom)). While all hypotheses identify between 95-100% of known actives, hypothesis D (red line in Figure 31(bottom)) performs best in identifying a large number of true positives while maintaining a low false positive rate. Hypothesis D in combination with a structure-based approach as described in IIb, will be used for virtual screening to identify potential additional antagonists of PKRs. Best candidates will be tested in functional assays in Prof. Meidan's lab.

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Dr. Masha Niv's group since 2007		
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Mor Rubinstein	PhD candidate	Volcani Institute
Dr. Shu Cheng	PostDoc	PostDoc in Université de Technologie de Compiègne, France
Yonatan Aizner	undergrad	MSc student at HUJI
Inbal Sela	project student	PhD student in Bar Ilan University
Anat Levit	PhD	current
Dr. Noga Kowalsman	PostDoc	current
Morin Shavro	MSc	current
Ayana Wiener	MSc	Current

Dr. Masha Niv scientific collaborations since 2007	
Name	Institution
Prof. Evgeni Ponimaskin	Hannover Medical School, Germany
Dr. Maik Behrens, Prof. Wolfgang Meyerhof	German Inst of Human Nutrition, Germany
Prof. Rob Coalson	University of Pittsburgh, US
Prof. Rina Meidan	HUJI
Prof. Daphne Atlas	HUJI
Prof. Micha Naim	HUJI

Dr. Masha Niv's grants since 2007			
Project	Period	Foundation	Total
Block Dynamics of Protein Kinases	2008-2010	BSF	40,000\$
Computational studies of AMPK	2007-2010	intramural	24,000\$
Computational and experimental analysis of oligomerization	2009-2012	Niedersachsen	109,000 euro
Bitter taste receptors	2008-	intramural	60,000 shekel
Biomolecular Simulations and Modeling - conference organization	2009	intramural	1000 \$

CONFERENCE ORGANIZATION

Biomolecular Modeling and Simulations - International Conference in Safed, Israel, 2009 initiator and member of the organizing committee

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Advances in Bioinformatics

ASSAF ZEMEL

RESEARCH ACTIVITY

Mechanical and geometrical features such as the cell shape and the rigidity of the surroundings were shown to play an important role in the regulation of central cellular processes such as cell proliferation and differentiation. The understanding of cellular mechano-sensitivity and of the molecular mechanisms involved in mechanical processes such as cell motility and division has been the subject of intense study in recent years. Our research focuses on several issues related to the mechanical activity and sensitivity of cells. We study the early stages of cell adhesion in which the cell shape and cytoskeleton structure establish. The consequences of these processes are believed to influence long term processes in the cell and to dictate the cell fate. On the molecular level, we study how ensemble of motor proteins and cytoskeletal filaments produce self-organization, movements and forces in the cell. Our initial work in this field concerned the sliding dynamics of microtubule and actin bundles that are cross-linked and powered by molecular motors; these bundles are common structures in many cellular processes

including cell division, muscle contraction and neuronal growth. Finally, we are also interested in understanding the collective response of ensemble of cells to elastic stresses produced either internally, by the contractile activity of the cells, or applied externally by forces such as blood pressure, muscle tension and gravity.

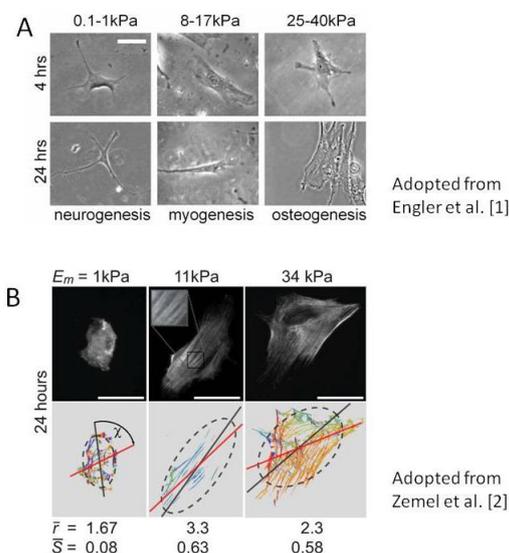


Figure 32: Human mesenchymal stem cells grown on substrates of varying rigidities. Panel A, shows the distinct cell morphologies that were obtained on the respective substrates, and Panel B, shows our analysis of the orientational distribution of the actomyosin stress-fibers in the cytoskeleton; see text and Refs. [1] and [2] for details.

CELL SHAPE, MATRIX RIGIDITY AND THE POLARIZATION OF STRESS-FIBERS IN CELLS

The motivation for this work has been the recent demonstration that the rigidity of the surroundings can direct the lineage specification of stem cells [1]. Cells plated on substrates of varying rigidities, that mimic that of brain, muscle and (pre-calcified) bone, were shown to differentiate to the corresponding tissue cell types after few days.

Interestingly, the shape that the cells adopted few hours after plated on the substrate resembled that of the mature cell type, namely of a neuron, muscle and bone cell on the respective substrates, as seen in the upper panel of . Quantification of the cells' aspect ratio showed that the cells optimally polarize on substrates of moderate (muscle-like) rigidity and obtain more isotropic structures on either soft or hard substrates. These findings suggest that the early time changes in cell shape due to cytoskeleton structure may play an important role in the long-term lineage specification process of stem cells.

To gain insight into the physical mechanisms involved in this important phenomenon, we focused on the alignment of the contractile, acto-myosin stress-fibers in the cytoskeleton of adhering cells that are thought to play an essential role in the active, mechano-sensitivity of the cell [2]. We demonstrated, both theoretically and experimentally, that the matrix rigidity regulates the polarization of stress-fibers in cells and dictates the preferential alignment of the stress-fibers along the long axis of the cell. In addition, we showed that the alignment of stress-fibers in stem cells depends non-monotonically on the matrix rigidity, attaining a maximum value for an optimal value of the matrix rigidity [2,3].

The cell was modeled as an active, elastic inclusion in an infinite, homogeneous and isotropic medium; we considered both two and three dimensional geometries. For simplicity the cell was assumed to have a spheroidal shape (ellipse in 2D) oriented with its long/short axis parallel to the z/x axis of a Cartesian coordinate system.

The theory included both the passive forces arising from the elasticity of the cell and the surrounding medium, as well as the active forces exerted and regulated by the cells; this extends the treatment of passive inclusions in solids [6, 7] to living matter. The active acto-myosin forces in the cytoskeleton were modeled by a local distribution of "force dipoles" [8–10] that arise from the equal and opposite forces exerted by myosin motors at two nearby points on actin filaments. These are represented by a tensor quantity $\langle p_{ij} \rangle$ which is the average (active) dipole density per unit volume. To relate the local polarization of the active forces in the cell to the local averaged stress, we invoked the use of an active cell polarizability as follows:

$$\langle p_{ij}^a \rangle = \langle p_{ij} \rangle - \langle p_{ij}^0 \rangle = -\alpha_{ijkl} \sigma_{kl}$$

where summation over repeated indices is implied. Here, $\langle p_{ij}^0 \rangle$, is the early time value of the average cellular dipole, $\langle p_{ij} \rangle$ is its actual value after the cell has polarized, and $\langle p_{ij}^a \rangle$ is the active polarization tensor. The (fourth rank) tensor α_{ijkl} is the cell polarizability tensor. This tensor couples (in an averaged and phenomenological manner) the active variations of the mean cellular dipole to the elastic stresses developed in the cytoskeleton. Refs. [2,3] discuss two forms of the polarizability tensor. One can show that for a particularly simple polarization mechanism, in which the forces polarize only parallel to the stress direction it is given by a simple scalar quantity, α .

The anchoring of a cell to the extracellular matrix as well as the active spreading on a surface, involve a global shape or volume deformation that produce elastic stresses in the cell and the matrix [11]. Our theory shows that for a cell that possesses some shape anisotropy, an isotropic adhesion-induced prestress in the cytoskeleton may initiate a spontaneous polarization of the stress-fibers. In addition, we find that the polari-

zation anisotropy (difference between stress-fibers aligned along the long axis and those oriented along the short axis of the cell) of the stress-fibers is maximal when the rigidity of the cell and the matrix are similar. In this range, the stress anisotropy resulting in the cell is most sensitive to the cell shape. Experiments were carried out to demonstrate this optimization using human mesenchymal stem cells plated on substrates of varying stiffness. The overall cell morphology was quantified in terms of the aspect ratio, r , and an analysis of stress-fiber formation and polarization was demonstrated for the first time by staining for actin and non-muscle myosin IIa.

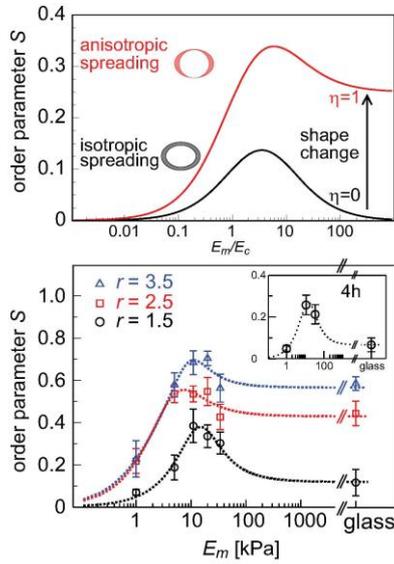


Figure 33: The effect of axial cell elongation on stress-fiber polarization and experimental values of the order parameter S for different elastic substrates; upper panel shows a calculation of the 2D order parameter as a function of the matrix rigidity, for two cases: the cell spreads isotropically on the substrate (black curve); the cell spreads anisotropically on the substrate (red curve). The two illustrations left of the curves show top views over the cell, before (shown as blank) and after (shown as shaded) cell spreading. In the asymmetric spreading case, r corresponds to the cell shape in an infinitely rigid matrix. For both curves we used $r=2$ and $\eta=1$. Lower panel shows the experimental values of the stress-fiber order parameter, 24 h after plating the cells, for the three groups of cells (of aspect ratios $r=1.5, 2.5$ and 3.5) as a function of Young's modulus of the matrix, E_m . Within each of the different groups, S is maximal for the 11 kPa matrix and generally increases with aspect ratio r , in agreement with our theoretical predictions. The error bars denote the standard error of the mean and theory curves (dotted lines) are shown to guide the eye.

The bottom panel of Figure 33 shows several representative images of cells, 24 hours after they were plated on substrates of Young's modulus, $E_m = 1, 11$ and 34 kPa. For comparison, the mean Young's modulus of the cell, E_c , was estimated by atomic force microscopy to be ≈ 10 kPa. The bottom row in that panel is the corresponding image analysis results, showing color-coded orientations of stress-fibers in the cell. The figure shows that stress-fibers optimally polarize on the matrix with intermediate rigidity, 11 kPa, as seen by the value of the orientational order parameter of the stress-fibers, $S = \langle \cos(2\theta) \rangle$; where θ is the angle of each stress-fiber from the long axis of a fitted ellipse. This parameter can be shown to be equal to $\langle p_{zz} \rangle - \langle p_{xx} \rangle / p$, where $\langle p_{zz} \rangle$ and $\langle p_{xx} \rangle$ are the diagonal elements of the polarization tensor and p is the trace.

Since our model treats the cell as an ellipsoid with given (and fixed) aspect ratio, r , the cells were sorted by their aspect ratio and the order parameter was evaluated for each group of cells separately. The bottom panel of Figure 33 shows the experimentally measured order parameter, S , as a function of the Young's moduli of the substrate E_m , for three groups of cells of $r = 1.5, 2.5, 3.5$. Theoretical curves (dashed lines) are shown to guide the eye. We find that for all cell shapes the orientational order parameter depends non-monotonically on the matrix rigidity showing a maximum for an intermediate value of the matrix rigidity. This non-monotonic dependence is more pronounced for the more rounded cells in the ensemble. For the more elongated cells (of aspect ratios 2.5 and 3.5), we find a shallower maximum and relatively high values of the stress-fiber polarization even at high values of the matrix rigidity. These observations can be explained as follows. Since in the early state of cell adhesion the cytoskeleton is still in an isotropic gel state, the elastic forces the cell exerts are likely to be isotropic. However,

even in this case our theory shows that for an intermediate value of the matrix rigidity, a small anisotropy of the cell shape may result in a breaking of symmetry of the elastic stress in the cell. This shape-induced stress anisotropy may feedback on the early-time force dipoles in the cytoskeleton, and cause a spontaneous orientation of the stress-fibers along the long axis of the cell. For either very high or very low matrix rigidity no stress propagates out of the cell (because in the former case the matrix is too soft to maintain a stress in the cell, and in the latter case the cell cannot deform the matrix) and hence the isotropic pulling forces of the cell result in an isotropic stress in the cell. We thus find a maximum of cell polarization on the matrix with moderate rigidity. Our experiments show that the more elongated cells polarize even when plated on very hard substrates. The upper panel of Figure 33 shows our theoretical predictions for the case that the cell spreads *isotropically* on the surface and exerts isotropic forces at early times (black curve), and for the case that the cell spreads *anisotropically* and exerts anisotropic forces on the substrate (red curve). We find that in the latter case the orientational order parameter shows a shallower maximum. We thus hypothesize that the concurrent elongation of the cells on the surface results in an axial contribution to the elastic stress in the cytoskeleton that in turn, is responsible for the polarization of the stress-fibers along the long axis of the cell. Our theory shows that this contribution increases monotonically with the matrix rigidity [2,3].

These findings unravel a fundamental and general relation between the cell shape, matrix rigidity and the polarization of stress-fibers in the cytoskeleton. The remodeling of the cytoskeleton architecture is an important consequence of cell adhesion. We believe that these processes are also responsible for the elastically-controlled modulation of the cell shape and spreading area on a surface as observed in experiments [3]. This provides physical insight into the mechanical mechanisms involved in the mechano-sensitivity of stem cell differentiation.

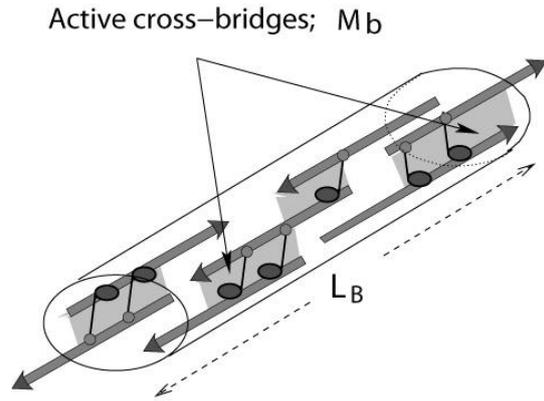


Figure 34: Schematic illustration of a cross-linked bundle of cytoskeleton filaments powered by molecular motors. M_b is the number of active overlap regions between filaments indicated by gray shading; L_B is the bundle length.

SLIDING DYNAMICS AND POLARITY SORTING OF ACTIN AND MICROTUBULE BUNDLES

Interactions of multiple molecular motors with bundles of actin and microtubule filaments form the basis for many cytoskeletal processes including axonal growth, muscle contraction, and cell division [14]. Continuum models based on generalized diffusion equations have been suggested to quantify the dynamics of such active bundles [15–17].

In highly cross-linked and densely packed filament bundles, however, a major complication arises due to the multiple interactions that each filament forms with its neighbors, see Figure 34. To theoretically explore the effects of these interactions on the self-organization and dynamics of the filaments we developed a computer simulation algorithm that allows us to calculate the velocities and the forces acting on the filaments in a self-consistent manner [18, 19]. We use a standard, linear force-velocity relation to relate the forces exerted by the motors to the velocity of the (pair of) filaments with which they interact. In a cluster of interacting filaments the forces exerted by the motors depend on the velocities of all the filaments in the cluster. This results in an algebraic set of equations for the forces on, and the velocities of the filaments. We

used our simulations to distinguish between different motor types at different densities and subject to different boundary conditions. We found that highly cross-linked bundles exhibit a percolation threshold beyond which the dynamics become strongly sensitive to the boundary conditions. In open bundles, interactions between multiple filaments result in significant acceleration of the filaments. In contrast, in ringed bundles, the long-ranged interactions between the filaments results in substantial slowing down of the filaments; in this case the motors behave as 'brakes' to the motion. The filaments in loosely connected bundles, on the other hand, undergo local diffusion-drift dynamics consistent with previous continuum models. Our simulations also demonstrate the sorting phenomena in the mixed-polarity bundles and reveal characteristic scales and conditions for spontaneous pattern formation in the bundle.

Figure 35 summarizes our results for the sliding-dynamics behavior in cylindrical bundles of $N = 100, 200, 300$ parallel filaments for different regimes of the motor density. The filaments are assumed to have a fixed length L . We compare two cases of boundary conditions: (i). periodic boundary conditions (mimicking a ringed morphology) and, (ii) an open bundle with absorbing boundary conditions on both ends of the bundle (i.e., filaments that reach the bundle edges 'fall' into solution); to compare the results with those of the previous case we assume that new filaments constantly nucleate at random positions to ensure a uniform and fixed density of filaments in the bundle. The relevant quantity that reflects the density of motors in the system and influences the dynamical characteristics of the filaments is the fraction of overlaps between neighboring pairs of filaments that are cross-linked by motors, $\chi_b = M_b / M$; where M is the total number of overlaps between filaments in the bundle and M_b is the number of cross-linked (bound) overlaps, see Figure 33. Panel a. shows the mean square velocity, $\sqrt{\langle v/v_0^2 \rangle}$, of the filaments (relative to the free velocity of the

motors v_0) as a function of χ_b for the two bundle morphologies. As expected, no boundary effects are observed for low densities of motors ($\chi_b = 0.1$); in this case only small clusters of filaments form in the bundle. At these concentrations, the filaments perform a random walk and long pauses are observed when the filaments remain unconnected to other filaments (panel b upper panel).

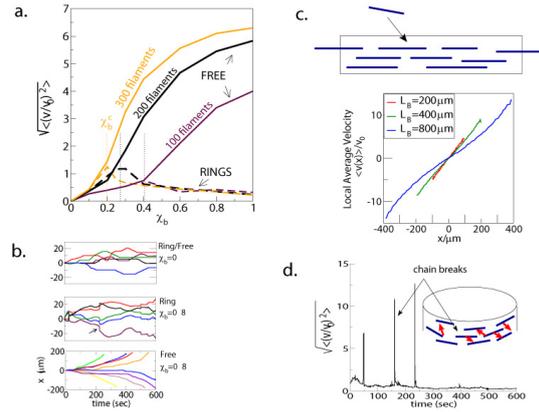


Figure 35: Dynamical characteristics of filaments in free (open) and ringed bundles of parallel filaments for different densities of (unipolar) motors. Panel a. shows the root mean square velocity as a function of the fraction of active overlaps between filaments, M_b . Panel b. shows several individual trajectories of filaments; upper section is for low motor density, middle section is for a ringed bundle at high density and lower section is for an open bundle at high motor density. Panel c. shows the velocity profile along the bundle (x -axis) resulting in a free bundle at high motor density. Panel d. shows a typical plot of the root mean square velocity as a function of time for a ringed bundle at high motor density.

At higher motor densities, we find qualitatively different dynamics once a threshold fraction of active cross-bridges is reached. This threshold fraction corresponds to a percolation transition in which interconnected clusters of filaments spanning the entire length of the bundle form. This percolation threshold is a property of the three-dimensional organization of the filaments in the bundle (hexagonal in a cross-section and spread along the bundle axis). The numerical value of the threshold fraction hence depends on the density of the filaments along the bundle length, N / L_B , and on the filament length L .

We find that $\chi_b^c \approx 0.3$; for comparison, the bond-percolation threshold is 0.34 for a two-dimensional triangular lattice and 0.25 for a three-dimensional cubic lattice [20].

When $\chi_b > \chi_b^c$, the behaviors of the open and closed (ringed) bundles are drastically different. In the free bundle with open edges, the filaments expand rapidly, with velocities that are few-fold higher than the free velocity of the motor (Figure 35a). The average filament speed increases with χ_b and saturates beyond the percolation threshold. Panel c shows the velocity profile of the filaments along the bundle (x-)axis. This graph shows that the filament speed increases toward the bundle edges. This behavior can be understood by examining a small cluster of interconnected filaments. In the absence of external forces, symmetry and momentum conservation ensure that the filament in the middle of the cluster is immobile. Filaments further away from the center move increasingly faster since they "piggy-back" on other moving filaments (this may be obtained quantitatively by solving the algebraic set of equations for the velocities of the filaments in the cluster, see [19]).

In contrast, in a ringed bundle, an increase in the fraction of active overlaps beyond the percolation threshold, $\chi_b > \chi_b^c$, results in a substantial slowing down of the motion. In this case the motors and filaments form closed chains in which the motors act as 'brakes' to the motion. Figure 35d shows an interesting behavior of dense ringed bundles of parallel filaments: once in a while, the closed interconnected filament chains get disconnected at random positions and open up. These transient events (appearing as spikes in Figure 35d) lead to very brief episodes of rapid sliding of the filaments.

FILAMENT SORTING AND PATTERN FORMATION IN THE BUNDLE

Since motor proteins always 'walk' in one unique direction, either the plus-or minus-end of a

filament, their activity results in spontaneous organization of the filaments. Figure 36 summarizes the results of our simulations for a long bundle ($L_B = 800 \mu\text{m}$) of filaments ($L = 10 \mu\text{m}$ long) consisted of an even mixture of filaments pointing in opposite directions. We consider both unipolar and bipolar motors as well as two regimes of the motor fraction parameter χ_b . Unipolar motors (e.g., dynein) comprise one 'walking' domain, and one 'cargo' domain with which they can anchor to a neighboring filament; a bipolar motor (e.g., myosin II) comprises two 'walking' domains. The generic difference between these two classes of motors is that while unipolar motors can slide apart two parallel filaments, bipolar motors don't; rather, these motors typically glide between parallel filaments at the maximum motor speed and exert no forces on the filaments. This inherent difference results in different sorting behavior of the filaments in the bundle. Interestingly, in some cases, which we describe below, the filaments in the bundle spontaneously cluster (on a time scale of tens of minutes) to form finite-size domains of parallel filaments whose polarity alternates along the bundle length.

The upper, pink/cyan colored sections in each panel show a projection of the bundle on the x-z plane, as obtained from the last time step (1.5 hours) in the simulation. Each pink/cyan bar represents a $10\mu\text{m}$ long filament and its color represents its orientation. Panels a. and b. show the behavior for unipolar motors (represented by one-headed blue arrows) and panels c. and d. are for bipolar motors (represented by two-headed yellow arrows). Upper panels are for low density of motors ($\chi_b = 0.1$) and lower panels are for high density of motors ($\chi_b = 0.8$). The graphs in each panel show the mean size of the domains as a function of time as calculated from the filament orientational-correlation-function, $C_n(d) = \langle n(d)n(0) \rangle$, where $n = \pm 1$ denotes the filament direction (as dictated by the walking direction of the motor on the filament) and the average (at a given time) is taken over all

filaments in the bundle and over an ensemble of trajectories with different starting configurations; d is the distance along the bundle axis between each given filament and any other filament in the bundle. The insets show $C_n(d)$ as a function of d for different time steps.

Typically, C_n is positive for small distances, negative for greater distances, and uncorrelated at large distances. This behavior implies that, on average, any filament in the bundle is surrounded by similarly oriented filaments in its vicinity and by oppositely oriented filaments at longer distances. The first zero of the correlation function is the average size of the domain [21]. Tracing the evolution of this size with time allows us to calculate the growth rate of the unipolar domains.

We find the following interesting behavior. Unipolar motors sort out the filaments at low densities (panel a.) but not at high densities (panel b.), while bipolar motors always sort out the filament and the rate of filament sorting increases with the motor density. In the case of unipolar motors at low density the pattern formation can be explained as follows. Interactions between antiparallel filaments typically result in fast directed motion of the filaments that leads to local sorting of the filaments (not shown). In contrast, interactions between parallel filaments in the unipolar domains that form, result in slower, diffusive motion that gradually increases the domain size. Whenever a filament of the opposite polarity moves into such domain, this filament rapidly drifts to a neighboring domain – this keeps the polarity separation. In contrast, densely connected bundles ($\chi_b = 0.8$) with unipolar motors remain homogeneously mixed and no ordering is observed as seen in Figure 36b. The explanation for this behavior relies on the formation of non-local interactions between the filaments whose outcome is a fast spreading of the filaments across the entire bundle length [19]. Similarly, bundles with bipolar motors (Figure 36c,d) self-organize to form periodic patterns, alas at both small and high motor density, because in this case non-local interactions do not

form in the bundle since bipolar motors do not exert forces on parallel filaments. The rate of the domain size growth increases with the bundle connectivity, χ_b , because in denser bundles, more motors shuffle the filaments more vigorously.

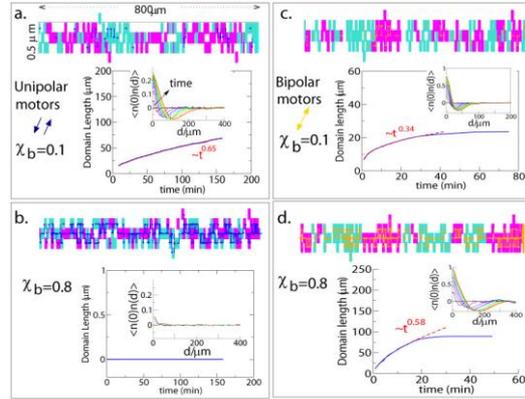


Figure 36: Polarity sorting and domain formation in bundles with an even mixture of filaments of opposite polarity. All simulations included a total of 400 filaments in an 800 μm long bundle that was subject to periodic boundary conditions. Right/Left panels are for bundles cross-linked by unipolar/bipolar motors; Upper/Lower panels are for low/high densities of motors. See text for details.

Finally, our simulations make important predictions about the self-organization and sorting of filaments in mixed bundles. In general, due to the inherent directionality of the motors on polar filaments a homogeneous mixture of filaments of opposite polarity is unstable and spontaneously sorts out to form intermittent clusters of filaments with opposite polarity. In biological systems, different levels of ordering are known to exist. In neurons microtubules are organized in parallel bundles while in dendrites and in proplatelets (the precursors of blood platelets) the microtubule bundles are mixed. The sarcomeric structure of muscle fibers and stress-fibers is yet another architecture of the filaments. Here actin filaments organize in a periodic manner forming alternating domains of filaments with opposite polarity. How these differences are maintained is still an open question. In the future we intend to continue our investigation of motor-filament interactions taking into account effects of applied forces and

INDIVIDUAL RESEARCH REPORTS

Assaf Zemel

bundling proteins and simulating these systems in higher dimensions.

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GRANTS

Israel Science Foundation: \$210,000, 2009-2013.

GROUP MEMBERS

- ❖ Leora Moshe – Ph. D student (2009)
- ❖ Roni Jutkowits - Ph. D student (2010)
- ❖ Einat Sagi – M.Sc student (2010)

COLLABORATORS IN GERMANY

- ❖ Dr. Florian Rehfeldt, III. Physics institute, Georg-August-University, Göttingen, Germany.
- ❖ Dr. Ralf Kemkemer, Max-Planck-Institute for Metals Research, Dept. New Materials and Biosystems, Stuttgart, Germany

PART II: CENTER ACTIVITIES AND BUDGET

INTRODUCTION

The scientific activity at the center has always been intense. Usually, about fifty scientists participate in this activity, including graduate students, post-doctoral fellows, visitors and faculty. There have been many added values to this activity, in addition to the many publications summarizing the research in the various groups. The Fritz Haber seminar, now running continuously for over twenty years, has become an "institution", hosting and attracting numerous scientists - from world leaders in their field to graduate students delivering their first public talk.

The center and its activities have attracted numerous young scientists to carry out their post-doctoral research or graduate studies at the Hebrew University. Over the years we have benefited from the presence of many dozens of post-doctoral fellows from Europe, the US and other countries around the world. Even during the difficult intifada times in Israel, and especially here in Jerusalem, there were several foreign post-doctoral fellows actively pursuing research at the Fritz Haber center.

Our many young excellent graduate students have always been an enthusiastic and exciting element in the center. Many of our former graduate students are now serving as senior scientists in various industrial companies, as well as in government and private research laboratories. Many others are among the leading scientists in academic institutes in Israel. Many are faculty members in leading foreign universities.

The center has a well established tradition of organizing and supporting scientific meetings in Israel on Molecular Dynamics and related fields, notably those where center members are involved in the organization (see appendix in part IV for details). To encourage theoretical chemistry research in Israel, The Fritz Haber Center has

initiated and organized a comprehensive theoretical chemistry conference (The first THEOCHEM meeting), which took place in Jerusalem in October 2002. This meeting has been a great success and has paved the way for more successful meetings since then. Several international meetings involving members of the center which took place afterwards are listed in Sec. 4.2 below. In particular, in March 2005, on the occasion of the Beirat meeting we held a special symposium on Biophysical Dynamics where, apart from several German and other distinguished speakers, most lectures were given by young faculty members from different Israeli institutes. This has been a very successful and inspiring meeting. In 2007 the center organized a Symposium on molecular conductance and supported many scientific conferences organized by its members (see appendix in part IV for details).

SYMPOSIA SUPPORTED BY THE CENTER (2004-2009)

The Center and Members have organized numerous international meetings and symposia since its foundation. The Center also supports, generally modestly, symposia in research fields related to its scientific activities; especially symposia involving the Center's members in the organizing committees, or as invited speakers. Below, is the list of meetings supported since 2003.

EIN GEDI WORKSHOP II: NON ADIABATIC PROCESSES AT SURFACES

Prof. Kosloff organized this symposium which took place at Ein Gedi, 11-15 January, 2004.

THE GENTNER SYMPOSIUM, IN HONOR OF PROFESSOR ERICH SACKMANN: PHYSICS OF BIOMATERIALS AND SOFT MATTER

Professor Ben-Shaul was a member of the organizing committee of this MINERVA - Gentner symposium, which took place in the Nirvana hotel, Dead Sea, March 14-17, 2004

SAFED WORKSHOP ON QUANTUM DISSIPATION

Professor Kosloff was a member of the organizing committee of this workshop which was held at the Hotel Merkazi in Safed, August 29 to September 4, 2004.

FRITZ HABER SYMPOSIUM ON BIOPHYSICAL DYNAMICS

Professors Kosloff and Agmon were members of the organizing committee of this workshop, which was held at the Jerusalem Mt Zion Hotel, March 13-14, 2005.

SAFED WORKSHOP ON QUANTUM THERMODYNAMICS

Professor Kosloff was on the organizing committee of this workshop which was held at the Hotel Merkazi in Safed, September 17-19, 2006.

TAIWAN-ISRAEL BINATIONAL MEETING: DYNAMICS ON MANY LENGTH (AND TIME) SCALES

Professor Levine was on the organizing committee of this bi-national meeting held at the Israel Academy of Sciences and Humanities in Jerusalem March 13-14, 2007.

FRITZ HABER DOUBLE-DAY SYMPOSIUM ON CONDUCTION IN MOLECULAR SYSTEM

Professors Baer and Kosloff organized this double-day symposium on conduction at Yad Hashmona, June 10-11, 2007.

SAFED WORKSHOP ON COOLING AND THERMODYNAMICS OF SYSTEMS

Professor Kosloff was on the organizing committee of this workshop which was held at the Hotel Merkazi in Safed, August 26-31, 2007.

SAFED SUMMER SCHOOL ON DENSITY FUNCTIONAL THEORY

Professor Baer was on the organizing committee of this workshop which was held at the Hotel Rimonim in Safed, September 1-6, 2007.

GENTNER SYMPOSIUM 2007 ON TIME DEPENDENT DENSITY FUNCTIONAL THEORY

Professor Baer was the chairman of the organizing committee of this MINERVA-Gentner Symposium. Hilton Queen of Sheba, Eilat 16-21 2007.

DIFFUSION, SOLVATION AND TRANSPORT OF PROTONS IN COMPLEX AND BIOLOGICALS SYSTEMS

Professor Agmon was a member of the organizing committee of this ISF workshop. Hilton Queen of Sheba, Eilat, January 13-17 2008.

BAT-SHEVA DE ROTHSCHILD SEMINAR ON ULTRAFAST-ULTRACOLD PROCESSES

Professor Ronnie Kosloff was a member of the organizing. February 24 - February 29, 2008.

1ST INTERNATIONAL SYMPOSIUM ON IMPROVED EXPLOSIVES

Organizer: Professor Kosloff, May 18 – 22, 2008. Venue: Rosh Hanikra Holiday Village.

FROM MACROMOLECULAR TO CELL BIOPHYSICS

Dr. Daniel Harries was a member of the organizing committee. June 3 - June 4, 2008.

SYMPOSIUM ON INTERFACES

Professor Roi Baer was the organizer May 25-26, 2009.

BIOMOLECULAR MODELING AND SIMULATION WORKSHOP

Organizers: Dr. Daniel Harries and Dr. Masha Niv. Safed, September 13 - 16, 2009

COMPUTATIONAL CHEMISTRY SYMPOSIUM

Organizers: Dr. Avital Shurki and Professor Roi Baer. Jerusalem, December 10, 2009.

GENTNER SYMPOSIUM ON PROTON MOBILITY IN CHEMICAL AND BIOLOGICAL SYSTEMS

Professor Noam Agmon is chair of the organizing committee. February 7 - 12, 2010 in Maagan Village.

A SYMPOSIUM IN MEMORY OF PROFESSOR VICTORIA BUCH

Organizer: Professor Roi Baer. May 10, 2010.

DEVELOPING TEACHING MATERIAL

For several years now, groups in the center have been developing unique teaching aids for quantum mechanics. The tools can be seen in the center website under the "Science Education" tab. The tools are Java 3D applets which describe many aspects of quantum mechanics in a way that is easily grasped by students and scientists. Here you will find applets that allow the manipulation of wave functions, their time evolution, calculation of correlation functions and even the Wigner distribution point of view.

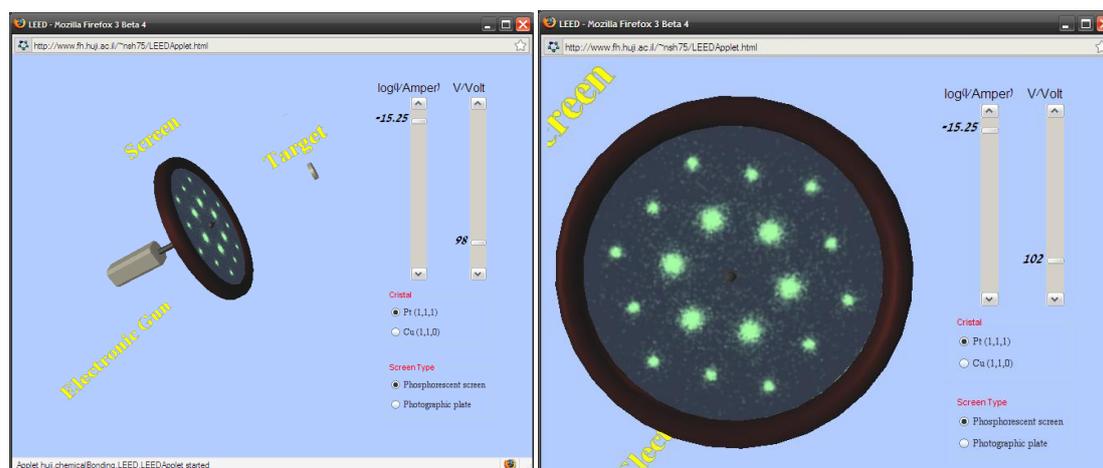


Figure 37: In this applet the simulation of a well known experiment, in which electrons accelerated by an electron gun, shot at a metal surface on which they impinge and scatter towards a fluorescent screen. A bright dot appears on the screen where an electron collided with it. The electron impingement continues at a rate determined by the student (the current/Amperes). The student can also control the velocity (Voltage/Volt) of the electrons. The applet is 3 dimensional so the students can rotate it and see the electron gun and the positions of the metal surface (right panel).

An example of an applet is described graphically in Figure 37. It simulates graphically a well-known experiment where electrons shot from an electron gun hit a metal surface and scatter onto a fluorescent screen. This applet teaches the students several basic concepts in quantum mechanics. First, particles such as electrons

have a wavy aspect since they exhibit interference pattern onto the screen. Second, the quantum mechanical wave function is a *probability amplitude* wave: the student can lower the rate electrons are shot at the screen and thus observe each electron separately as it impinges on the screen in a random location, un-

correlated with the other electrons. The student will see that some points on the screen are brighter than others. These brighter spots are formed when many electrons tend to impinge at the locations where the wavefunction has maxima. Third, the interference pattern of bright spots toggles between hexagonal to square when the student switches the metal surface serving as a grating from Platinum to Copper. Fourth, the student can study the de-

Broglie relation $p = h/\lambda$ between the particle aspect, namely the "momentum" p , and the wavy aspect, namely the "wave length" λ (the constant h is "Planck's constant"). By changing the velocity of the electrons shot at the screen, the student can explore the relation between velocity and the distance between bright spots which reflects the wave length.

PART III: STATUS REPORT DECEMBER 2009

PERSONNEL

MEMBERS OF THE CENTER

- N. Agmon, Ph.D., Professor of Theoretical Chemistry
- R. Baer, Ph.D., Professor of Theoretical Chemistry
- A. Ben-Shaul, Ph.D., Sherman Professor of Theoretical Chemistry
- V. Buch, Ph.D., Professor of Theoretical Chemistry (until her passing away on June 2009).
- R.B. Gerber, D.Phil., Fiedler Professor of Chemistry
- D. Harries, Ph.D., Senior Lecturer of Theoretical Chemistry
- R. Kosloff, Ph.D., Sonneborn Professor of Theoretical Chemistry
- R.D. Levine, Ph.D., D.Phil., Max Born Professor of Natural Philosophy
- Masha Y. Niv, Ph.D., Senior Lecturer
- Assaf Zemel, Ph.D., Senior Lecturer

THE RESEARCHERS AT THE CENTER

There are about 60 scientists at the Center, including professors, long-term visitors, post-doctoral fellows and graduate students. Two system managers are responsible for the maintenance and frequent upgrading of the diverse computing facilities of the Center and those of its members.

SCIENTIFIC (NON-FACULTY) STAFF

- Dr. Brina Brauer
- Dr. Faina Dubnikov
- Dr. Tova Feldman
- Dr. Gil Katz

LONG TERM VISITING SCIENTISTS 2008/9

- Prof. A. Dell-Hammerich (University of Illinois)
- Prof. F. Remacle (University of Liege)
- Prof. D. Neuhauser (UCLA)
- Dr. Madeleine Pincu (UCLA)
- Dr. Eyal Fatal, Biological Institute, Israel
- Dr. Shlomi Pistinner, Soreq Research Center.
- Dr. Naomi Rom, Rafael Technologies.

POSTDOCTORAL FELLOWS AND RESEARCH ASSOCIATES (2008/2009)

- Dr. Saieswari Amaran
- Dr. Shu Cheng
- Dr. L Cwiklik
- Dr. B. Cwiklik
- Dr. Helen Eisenberg
- Dr. Jennifer Galanis
- Dr. Noga Kowalsman
- Dr. Moshe Goldstein
- Dr. Rebecca S. Granot
- Dr. Shimshon Kallush
- Dr. Chen Levi
- Dr. Esther Livshits
- Dr. Soohyung Park
- Dr. Jiri Sebek
- Dr. Dorit Shemesh
- Dr Michal Steinberg

- Dr. Iad Suan

RESEARCH STUDENTS 2008/2009

Amshallem, M., PhD, Bar, L., PhD., Baratz A. PhD, Brill, Y., PhD, Buchman, O. PhD, Cnaani R PhD, Gershon, T PhD, Hirshberg B., BSc., Jacoby S. PhD, Jutkowits R PhD, Klein, M., PhD, Levit A PhD, Levy A. MSc, Moshe L, MSc, Muscatal, H. PhD, Polity, R., PhD, Razek, Y., PhD, Rubinstein M PhD, Safer G., MSc, Sagi E. MSc, Sagiv L. PhD, Sapir L MSc, Schafer I. MSc, Shachar A. N., MSc, Shavro M MSc, Shinobo, Ai, MSc, Shmiloviz-Ofir PhD, M., Shudler M MSc, , Sukenik, S. MSc, Tsvik Y BSc, Tzivyon, U.O., PhD, Wiener A MSc, Zmiri, L. MSc.

ADMINISTRATIVE-TECHNICAL STAFF

The center's administrator is Ms. Geula Levy who is in charge of the smooth operations of the center. The entire administrative work at the center which involves following up and allocating funds to the many budgetary items, the purchase of equipment, taking care of all the visitors and students, and coordinating these activities with the Hebrew University's administration - all this workload is shouldered most efficiently by Ms. Levy.

Mrs. Eva Guez, the center's secretary since its inception, has retired in September 2001. Eva is still helping us on a part time basis, including in the preparation of this report.

Our complex and diverse computing services are taken care of by a professional system manager helped by a part time assistant system manager. The current system manager are Mr. Michael Vilenkin, who performs an excellent job in maintaining and upgrading our computational infrastructure. Most valuable help in maintaining and developing the computing facility in the center is provided by Mr. Max Tkach, who works at the center half time.

The Institute of Chemistry supports the basic salary of the system manager (Mr. Vilenkin). The part time system manager assistant; extra hours, travel expenses and many other benefits are paid from the center's budget.

CENTER COMPUTING RESOURCES

The computer facility of the Center is the principal research tool of all scientists in the center. Most of the computers are purchased by the different researchers from their personal grants. The center offers to the researchers the services of a System Manager and his assistant.

Mr. Michael Vilenkin, and Mr. Max Tkach are responsible for the maintenance and development of our computer services, which include both equipment of the Center, and machines used by individual groups. Computational research activities in all the groups depend heavily on the smooth functioning of the unit. This team also maintains the webpage of the center.

NUMBER-CRUNCHING RESOURCES

There are currently over 250 computer cores, mostly Intel 64 bit machines running Linux. These are grouped in 7 distributed memory clusters, owned by the different members of the centers but managed by the System Administrator. Some of the clusters are connected to the university grid by the MOSIX software developed by Professor Amnon Barak from our computer science department. Additionally a strong SGI shared memory computer with 8 2-CPU diskless nodes Itanium-II processors with 64GB shared memory and a single system image has been purchased.

OTHER USER SERVICES

The computer services were based on a 10-disk RAID protected storage system, with about 1.5 Terra-byte volume. This server provides shared program access, YP authorization, home directory services and POP/IMAP mail services, printing, group website hosting etc. This server has failed

Part III: Status Report

twice at the end of 2007 and we have decided to replace it with a new system in 2008. In parallel we also maintain two Windows 2003 domain servers with 450 GB disk space that provide active directory services, terminal services (remote desktop), such as DNS, authorization, home directory, FTP, printing, virus protection. of shared storage for the various users of Windows. In addition we have Mac-OS workstation connected

to the Center Linux authorization system. All the clusters, workstations and servers are connected by switched 100Mb Ethernet with a 1Gb backbone network. Laptop owners can use the university installed wireless connection network with a 54Mb speed.

PART IV: APPENDICES

LIST OF VISITORS AND SEMINARS 2004-2009

Below we list the visitors and speakers in the Fritz Haber seminars during the period 2003-2007. We also mention the numbers of scientists attending the various workshops and symposiums which the center has organized in this period.

Date	Speaker	Title
1.1.04	Prof. G. Kurizki, Weizmann Inst.	Manipulation of Entanglement and Decoherence in Molecules
8.1.04	Prof. E. D. Tannenbaum, Harvard University	Semiconservative Replication in the Quasispecies Model
11-15.1.04	EIN-GEDI WORKSHOP Non-Adiabatic Processes on Surfaces Organizers: M. Asscher, E. Kolodney, R. Kosloff & Y. Zeiri	Non-Adiabatic Processes on Surfaces Organizers: M. Asscher, E. Kolodney, R. Kosloff & Y. Zeiri Dr. H.L. Abbott, University of Virginia: Vibrational State Resolved Dissociative Chemisorption of Methane on Ni(100) Prof. D. Auerbach, Hitachi Technologies: Probing Nonadiabatic Coupling in Molecular Interaction with Surfaces Prof. R. Baer, HU: Electronic Processes and Transition on Surfaces - A Time Dependent Density Functional Approach Prof. L.S. Cederbaum, Heidelberg: Beyond Born-Oppenheimer: Molecular Dynamics Through A Conical Intersection Prof. D. Chakarov, Goteborg, Sweden: Photo Physics and Photo Chemistry of Ice Films on Graphite Dr. M.P. de Lara-Castells, Inst. de Mat. y Fisica Fundamental, Madrid, Spain: Nonadiabatic Effects in the Light-Induced Desorption of O2 from the TiO2 (110) Surface Prof. V.A. Esaulov, Lab. des Collisions Atom. and Molec. Universite de Paris Sud, France: Electron Transfer Prozesse in Ion/Atom Scattering on Surfaces Prof. H.-J. Freund, Chem. Phys., Max Planck, Berlin: Photodesorption from Oxides and Deposited Metal Clusters: REMPI and 2PPE Investigations Prof. J.W. Gadzuk, NIST, Gaithersburg: Production and Deterction of Chemically-Induced Hot Electrons in Surface Processes: X-Ray Edges, Driven Oscillators, Friction Dr. E.D. German, Technion: Theory of Dissociative Adsorption Kinetics of Diatomic Prof. A. Gross, Physik Dept., TU Muenchen: Multidimensional Mixed Quantum-Classical Description of the Laser-Induced Desorption of Molecules Prof. I. Harrison, University of Virginia: Photoinduced Electron Transfer Chemistry and Dissociation of Adsorbed CO2: Harnessing A-Scale Molecular Acceleration Towards a Sur-

		<p>face</p> <p>Prof. E. Hasselbrink, Chem., Duisburg-Essen: Non-adiabatic Pathways in the Dissociative Adsorption of Simple Molecules in the Al(111) Surface Prof. U. Hoefer, Physic Dept, Philipps Univ., Marburg:</p> <p>Time-Resolved Two-Photon Photoemission of Ar/Cu-Interface States Prof. S. Holloway, Surf. Scie. IRC, Univ. of Liverpool: Dynamics of Spin Transition in the Adsorption of Hydrogen Atoms on Metals Prof. A. Hoffman, Technion: Initial Stages of Oxygen Adsorption on Al(100) Surfaces Studied by Photoelectron Spectroscopy and Low Energy Ion Scattering Dr. S. Jorgensen, Inst. of Chemistry, HU: Adsorbate Orientational Dependent Photoinduced</p> <p>Desorption of CH₃Br on Ru(001) Dr. A. Kaplan, Technion & University of Birmingham: Implanting Atomic Ions into Surface Adsorbed Fullerenes: The Single Collision Formation and Emission of Endohedral Complexes Prof. B. Kasemo, Chalmers and Goteborg University: Spontaneous and Photo-induced, Non-adiabatic Processes on Extended and Nanoscale Surfaces Dr. G. Katz, Fritz Haber, HU: Abstractive Dissociation of Oxygen Over Al(111): A Nonadiabatic Quantum Model Dr. Th. Kluener, FH Inst., Berlin:</p> <p>Theoretical Investigation of Photochemical Reactions on Surfaces from First Principles Prof. A.C. Kummel, UC San Diego: Hyperthermal Ejection of Halogen Atoms from the Reaction of Diatomic Halogens on the Al(111) Surface: Evidence of A Vertical Electron Harpooning Mechanism Dr. Y. Lilach, HU:</p> <p>Steric Effect in Electron-Molecule Interaction Prof. D. Menzel, TU Munich: Ultrafast Charge Transfer and Localized Bond Breaking at Surfaces Prof. N. Moiseyev, Technion: Trapping of Electrons Due to Nonadiabatic Processes Prof. R. Naaman, Weizmann Inst.: Surprising Electronic Properties of Two Dimensional Chemical Systems Prof. A. Nitzan, Chemistry, TAU: Timescale Considerations in Electron Transfer and Electron Transmission Dr. I.D. Petsalakis, Theoret. and Phys. Chem. Inst., National Hellenic Research Foundation, Athens: Theoretical Study of Adsorption of Halogen-Substituted Benzene on a Si(111) Surface Prof. U. Peskin, Technion, Haifa: Modulations of Electronic Tunneling Rates</p> <p>Through Flexible Molecular Bridges by a Dissipative Super-Exchange Mechanism Prof. P. Saalfrank, Chemistry, University of Potsdam: Quantum Dynamics of Non-Adiabatic Processes at Surfaces Dr. B. Segev, BG University, Beer Sheva: The Evanescent-Wave Mirror for Cold Atoms</p>
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Part IV: Appendices
List of Visitors and Seminars 2004-2009

		<p>Prof. T. Seideman, Chemistry, Northwestern University: Nonadiabatic Vibronic Dynamics as a Tool. From Surface Nanochemistry to New Forms of Molecular Machines Dr. G. Theodorakopoulos, Theoret. and Phys. Chem. Inst., National Hellenic Research Foundation, Athens: Theoretical Study of Reactions of Benzene and Dibromobenzene at a Si(111) Surface Prof. M. Wolf, Freie Univ. Berlin: Ultrafast Dynamics of Non-adiabatic Processes at Interfaces: From Surface Femtochemistry to Coherent Phonon Excitation Prof. Xiaoyang Zhu, Univ. of Minnesota: Understanding Electron Transfer at Molecule- Metal Junctions: A Spectroscopic Approach</p>
29.1.04	Dr. A. Vardi, BG University	Second-sound Solutions in Ultracold Gases
15-31.1.04	Prof. T. Seideman, Chemistry, Northwestern University:	Nonadiabatic Vibronic Dynamics as a Tool
14-28.2.04	M. Kjellberg,	
24.2-23.3.04	Dr. Ch. Koch, CNRS, Paris	Formation of Ultra Cold Molecules
4.3.04	Dr. E. Pazy, BG University	pin-Based All-Optical Quantum Computation employing Semiconducting Quantum Dots
5-19.3.04	Prof. W. Rethig,	Photochemistry of Excited State Reactions
14-17.3.04	<p>GENTNER SYMPOSIUM on The Physics of Biomaterials and Soft Matter Nirvana Hotel, Dead Sea. Organizers: D. Andelman (TA), A. Ben-Shaul (J'lem), S. Safran (Weizmann) T. Bayerl (Wurzburg), H. Gaub (Munich), R. Lipowsky (Golm) and H. Mohwald (Golm)</p>	<p>Session I: Physics of Cell Adhesion (R. Lipowsky, Chair) P.G. de Gennes (Curie): Adhesion and Friction of Soft Objects and/or cell Motions B. Geiger, (Weizmann): Mechanosensitive Interactions Association with Cell Adhesion and Migration R. Merkel (Julich): Kinetics of Single Bonds Under the Influence of Piconewton Forces D. Roux (Bordeau): Adhesion of Colloids on Cells U. Seifert (Stuttgart): Pulling on Biopolymers, Adhesion Patches and Vesicles: Theoretical Case Studies about the Effect of Forces in Model Systems M. Tanaka (Munich): Polymer Supported Membranes as Bio-functional Interfaces and Cell Surface Models M. Kozlov (Tel-Aviv): Focal Contacts as Mechanosensors: A Thermodynamic Model Session II: DNA Physics(H. Gaub, Chair) A. Minsky (Weizmann): Physical and Structural Aspects of DNA Repair: Role of Restricted Diffusion E. Braun (Technion): From DNA to Transistors by Sequence-Specific Molecular Lithography W. Helfrich (Berlin): Electro-Optically Switchable Columnar Liquid Crystals: Modeling and Conjectured Structure Session III: Cytoskeleton and Actin(H. Mohwald, Chair) E. Sackmann (Munich): Micro-viscoelasticity of Cells F. Mackintosh (Amsterdam): Elastic Response of Cytoskeletal Net-</p>

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List of Visitors and Seminars 2004-2009

		works N. Gov (Weizmann): Cytoskeletal Control of the Red-Blood Cell Membrane C. Safinya (UCSB): Supramolecular Assembly of Biological Molecules: From Physics to Biomedical Applications E. Frey (Berlin): Statistical Mechanics of the Cytoskeleton - Fiber Networks and Intracellular Transport J. Radler (Munich): Bits and Pieces - From Vesicles to Cell Motion A. Bernheim (Ben Gurion): Biomimetic System for the Study of Actin Based Movement Session IV: Macromolecular Assemblies(T. Bayerl, Chair) A. Bausch (Munich): Spherical Crystallography W. Gelbart (UCLA): What is the Pressure in a Virus, and Why? R. Bruinsma (UCLA): Origin of Icosahedral Symmetry in Viruses H. Strey (Amherst): Nanoporous Materials for Biomedical Applications I. Arkin (Jerusalem): Membranes Containing SARS Coronavirus Proteins S. May (Jena): Protein-Induced Demixing of Charged, Binary Lipid Membranes Session V: Dynamics of Biomaterials (J. Klein, Chair) F. Brochard (Curie): Vesicles: Transient Pores and Nanotubes R. Granek (Ben Gurion): Dynamics of Biopolymer Systems in and out of Equilibrium U. Schwarz (Golm): Stochastic Dynamics of Leukocyte Tethering in Shear Flow H. Diamant (Tel Aviv): Hydrodynamic Interactions in Confined Suspensions
17-21.3.04	S. May (Jena)	Beyond Born-Oppenheimer: Molecular Dynamics Protein-Induced demixing of Charged, Binary Lipid Membranes
23-26.3.04	Prof. L.S. Cederbaum, Heidelberg:	Beyond Born-Oppenheimer: Molecular Dynamics
1.4.04	Dr. S. Keinan, Chemistry, Northwestern	Computational Design of Materials
29.4.04	Prof. F. Stoddart, UCLA	An Integrated Systems-Oriented Approach to Molecular Electronics
6.5.04	Dr. H. Diamant, Chemistry, TAU	Confinement Effects on Colloidal Dynamics
20.5.04	D. Gelman, HU	Quantum Dynamics of Fast Dissipative Processes
27.5.04	A. Zemel, HU	Membrane Perforation Induced by Amphiphatic Peptides
28.5-2.6.04	Prof. J. Manz, FU Berlin	Coherent Spin Control: Model Simulations for Dihalogenes in Rare-Gas Matrices
3.6.04	Prof. A. Brokman, HU	Critical Morphological Transition by Elastic Interaction
4-11.6.04	Prof. P. Devlin, Oklahoma State Univ.	Ice Surface Structure
9.6.04	Dr. M. Leibscher, FU Berlin	Controlling Quantum Rotation: Atom Squeezing and Molecular Alignment
2-6.7.04	Prof. J. Heath, Caltech	Molecular Mechanics and Electronics
1-5.8.04	Prof. H. Schubert, Fraunhofer Inst. Pfinztal	Explosives
30.7-	Prof. J. Oxley, Rhode Island	Explosions: Explosives Not Required

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List of Visitors and Seminars 2004-2009

6.8.04		
12.8-10.9.04	Dr. Ch. Koch, CNRS, Paris	Formation of Ultra Cold Molecules
29.8-3.9.04	SAFED WORKSHOP on QUANTUM DISSIPATION Open Problems in Open Quantum Systems Organizers: R. Kosloff (HU) and D. Tannor (Weizmann) R. Kosloff (HU): Markovian Master Equation (Lindblad Form) D. Tannor (Weizmann)	Markovian Master Equation R. Coalson (Pittsburgh): Spin-Boson Dynamics U. Kleinekathofer (Berlin): Markovian Master Equation E. Rabani (Tel-Aviv): Quantum Mode-Coupling Theory E. Geva (Michigan): Classical Quantum Methods E. Pollak (Weizmann): Classical Methods R. Kosloff (HU): Surrogate Hamiltonian Method D. Cohen (Beer-Sheva): Quantum Dissipation and Classical Chaos A. Nitzan (Tel-Aviv): Molecular Conduction U. Peskin (Technion): Electron Transfer U. Kleinekathofer (Berlin): Stochastic Unravelling and Exciton Transfer D. Tannor (Weizmann): Non-Markovian Master Equation D. Cohen (Beer-Sheva): Driven Systems/Kubo N. Moiseyev (Technion): Non-Hermitian Quantum Mechanics R. Coalson (Pittsburgh): Driven Systems E. Geva (Michigan): Driven Systems Y. Imry (Weizmann): Decoherence and Noise Correlators in Mesoscopic Systems
29.8-23.9.04	S. Dittrich, FH Inst. Berlin	Surface Science
21.10.04	Dr. B. Davidovitch, Harvard Div. of Eng. and Appl. Sci.	Continuum Approach in Studying Nano-Scale Surface Phenomena
25-26.10.04	Dr. E. Tannenbaum	Modeling Vibrational Predissociation of the van der Waals Complex ArHF
28.10.04	Dr. D. Barash, Computer Sci., Ben Gurion Univ.	Computational Prediction of Mutations Causing RNA Switches
3-29.11.04	Dr. J. Palao, University of La Laguna, Spain	Quantum Molecular Coupling
4.11.04	Dr. E. Pazy, Chemistry, BG University	Making Bosonic Molecules from Fermionic Atoms Employing Feshbach Resonances: The Importance of Symmetry Considerations
11.11.04	Dr. O. Alon, Heidelberg	Effective Orbitals for Complex Problems Methods and Applications
25.11.04	Prof. P. Zdanska, Organic Chem. and Biochem.	Academy of Sciences, Czech Republic Statistical Interpretation of Complex Scaling Method
29.11-6.12.04	Prof. J.P. Devlin, Oklahoma State University	Ice Surface Spectra
4-18.12.04	Dr. S. Jorgensen, Aarhus University, Denmark	Single Molecular Reactions on Cold Molecular Ions
7-25.12.04	Dr. A. Yoffe, UCLA	Phenomenological Model - Size and Shape of the Single-Stranded Viral RNA Genome Single-Stranded Viral RNA Genome
14-16.12.04	Prof. R. Grimm, Innsbruck University, Austria	Laser-Atom Interactions
16.12.04	Prof. M. Drewsen, Physics and Astronom., Aarhus University	Cold Molecular Ion Studies in Traps
30.12.04	Prof. D. Lidar, Univ. of Toronto	Two Problems in the Theory of Open Quantum Systems Post-Markovian and Adiabatic Quantum Dynamics

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List of Visitors and Seminars 2004-2009

4.1.05	Prof. A. Mogilner, UC Davis	Multiscale Two-Dimensional Modeling of Migrating Keratocyte Cells
25.2-3.5.05	Dr. M. Guehr, Freie Univ. Berlin	Coherent Dynamics of Small Molecules in Rare Gas Crystals
3.3.05	Dr. V. Averbukh, Heidelberg	Interatomic/Intermolecular Coulombic Decay in Clusters: From Diatomics to Fullerenes
8.3.05	Prof. T. Saue, Louis Pasteur University, Strasbourg	4-Component Relativistic Density Functions Theory
13-14.3.05	The Fritz Haber Symposium on Biophysical Dynamics, Mt. Zion Hotel, Jerusalem	Prof. G. Comsa (Bonn), Participant (Beirat) Session I: Biodynamics. Ronnie Kosloff, Chair Prof. H. Gruebmuller, Goettingen Elaborate pores and complex machines: Nature's nanotechnology benchmarks Victoria Buch: Computational studies of ether-acid solids Gilad Haran: The chemical physics of protein folding and association: Single molecules and more Session II : Benny Gerber, Chair Yossi Klafater: Single molecule dynamics: An enzyme case Nir Gov: Physics of active membranes and cytoskeleton Haim Diamant: Folding cascades in a compressed lipid monolayer Session III: Avinoam Ben-Shaul, Chair Noam Agmon: Proton pathways in green fluorescent protein Natalie Questembert-Balaban: Soft lithography for quantitative studies of biological systems Raphy Levine: Molecular logic machines and DNA computing Session IV: Roi Baer, Chair Misha Koslov: Elastic mechanism of processive capping of actin filaments by formins Nir Ben-Tal: Dynamics of peptide adsorption onto- and insertion into- membranes Shelly Tzlil: Flexible macromolecule-membrane interaction and viral budding Leonid Chernomordik: Membrane fusion: Pathways and inhibitors Session V: Victoria Buch, Chair Anne Bernheim: Formation pathway to aster and stars by actin polymerization Assaf Friedler: Biophysical studies of the tumor suppressor protein p53: A tool for the development of anti- cancer lead compounds Simha Srebnik: Adsorption behavior of model proteins embedded in a polymer brush Session VI: Noam Agmon, Chair Benny Gerber: Vibrational spectroscopy and the development of novel force fields for biological molecules Sandy Ruhman: Ultrafast spectroscopic studies of bacteriorhodopsin Wolfgang Domcke: Hydrogen bonds, conical intersections and photostability of life.
17.3.05	Dr. E. Brown, UCI Molecular Spectroscopy of Atmospheric Systems:	Predictions from Molecular Dynamics Simulations
7.4.05	Prof. F. Masnou-Seeuws, Lab. Aimée Cotton, Orsay Photoassociation of Cold Atoms with Chirped Laser Pulses	Correlation Effects in Coupled Atomic-Molecular Condensates
7-13.4.05	Prof. J. Sadlej, University of Warsaw	Quantum Chemical Calculations of Spectroscopic

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List of Visitors and Seminars 2004-2009

		Effects
8-14.4.05	Dr. N. Uras-Aytemiz	Acid Hydrate Phases in Nanoparticles
9-17.4.05	Dr. A. van Duin, Caltech ReaxFF,	A Transferable Computational Method for Atomic Scale Dynamical Simulations of Chemical Reactions
14.4.05	Prof. F. Brown, Chemistry,	UCSB Simplified Models for Biomembrane Structure and Dynamics
19.4-5.5.05	Dr. U. Poschinger, Physikalisches Inst., Freiburg	Ultra Cold Molecules
3-11.5.05	Prof. P. Devlin, Oklahoma State University	Ice Surface Spectra
17-31.5.05	Prof. L. Diosi, Particle and Nucl. Phys. Inst., Budapest	Quantum Thermodynamics
19.5.05	D. Shemesh, HU Photoionization of Biological Molecules:	Conformation Selective Processes
19-24.5.05	Prof. W.D. Phillips, NIS, Gaithersburg	A Bose-Einstein Condensate in an Optical Lattice Atomic Physics Meets Solid State
26.5.05	Y. Miller, HU	Vibrational Spectroscopy and Photoinduced Reaction Dynamics of Atmospheric Molecules
31.5-9.6.05	Prof. M. Gordon, Iowa State University	Potentials for Solvent Effects and Beyond
8.6.05	Prof. M. Ratner, Northwestern University	Molecular Transport Junctions: Scattering, Disorder and Vibronics
8-10.6.05	Prof. H. Schubert, Fraunhofer Inst., Pfinztal	Explosives
8-11.6.05	Prof. J. Oxley, Rhode Island	Explosions and Explosives
9.6.05	Prof. I.B. Bersuker, Theoretical Chem., Univ. of Texas at Austin	The Jahn-Teller Effect as a Unique Mechanism of All The Symmetry Breakings in Molecular Systems and Condensed Matter
10.11.05	Dr. I. Averbukh, Weizmann Institute	Optical Kicking: Laser Control of Molecular Orientation
17.11.05	Dr. S. Kallush, Fritz Haber, Hebrew University	The Quantum Governor: Automatic Quantum Control and Reduction of the Influence of Noise Without Measuring
24.11.05	Prof. J.M. Gordon, Ben Gurion University	Solar Photonics for Applications in Medicine, Power Generation and Nanomaterial Synthesis
1.12.05	Dr. N. Gov, Weizmann Institute, Rehovot	Active Motion and Structural Phases of Cell Membranes
9-14.12.05	Dr. S. Karthausser, Center for Nanoelectronic Systems for Information, Technology, Jülich	Resistive Switching
8.12.05	Dr. V. Teif, Inst. Biorg. Chem., Belarus Acad. Sci.	Lattice Models for DNA-Ligand Binding
15.12.05	Dr. C.P. Koch, The Fritz Haber, Hebrew University	Making Ultracold Ground State Molecules with Optical Fields
22.12.05	Dr. D. Cohen, Physics Dept., Ben Gurion University	Linear Response, Absorption of Radiation by Small Conducting Particles, Conductance of Mesoscopic Devices
2.1.06	Dr. I.N. Berezovsky, Chemistry, Biol. Chem., Harvard	Physical Origins and Evolution of Protein Stability and Adaptation
5.1.06	Dr. V. Teif, Bio-Organic Chem. Inst., Belarus Nat. Acad. Sci., Minsk	Lattice Models for DNA-Ligand Binding
8-19.1.06	Dr. U. Poschinger, University of	Cold Molecule Formation

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List of Visitors and Seminars 2004-2009

	Freiburg	
12.1.06	Prof. N. Agmon, HUJI	The Remarkable Dynamics of the Green Fluorescence and its Chromophore
16-19.1.06	Prof. V. Vaida, Chemistry Dept, University of Colorado	Chemical Reactivity – Light Induced Chemical Reactions
19.1.06	Dr. S. Zilberg, Physical Chem., HUJI	Design of the Singlet-Triplet Bistable System
23-31.1.06	Dr. N. Uras-Aytemiz, Chemistry, Oklahoma State University	HCl Solvation at Surface and within Methanol Clusters/Nanoparticles
26.1.06	Dr. K. Solntsev, Georgia Inst. of Technol., GA	Excited-State Proton Transfer: From "Super" Photoacids to the Green Fluorescent Protein
2.2.06	Prof. O. Biham, Racah Inst. of Physics, HUJI	Molecular Hydrogen Formation and Complex Reaction Networks on Dust Grains in the Interstellar Medium
19-24.2.06	Dr. K. Breuker, Inst f. Organic Chem. & Center f. Molecular Sciences, Innsbruck, Austria	Electrons for the Structural Characterization of Proteins in the Gas Phase
28.2-3.3.06	Prof. A. M. Wodtke, Chemistry & Biochemistry, UCSB	The "Standard Model" of Chemical Reactivity: How Well Does It Describe Reactions at Metallic Interfaces
8.3.06	Prof. R.D. Levine, Physical Chem. & FH Center, Hebrew University	Is There an Electronic Time Scale in Chemistry
16.03.06	Prof. P. Jungwirth, Czech Academy of Sciences	Solvation of Ions at Aqueous Interfaces
	Dr. S. Jorgensen, Dept of Physics & Astron., Aarhus University, Denmark	Controlling Reaction Dynamics
23.03.06	Prof. A. Millet, Universite Joseph Fourier, Grenoble	Theoretical Studies of Organometallic Reactivity: Pauson-Khand Reaction and Reductive Elimination from Octahedral Pt(IV) Complexes
30.3.06	Prof. A.I. Burshtein, Chemical Physics, Weizmann Institute	Non-Markovian Chemical Kinetics
30.3-3.4.06	Prof. B. Andresen, Niels Bohr Inst., University of Copenhagen	Fuel Cells and Finite-Time Thermodynamic Optimization of Mitochondrial Chemistry
6.4.06	Dorit Shemesh, Fritz Haber Inst. & Dept of Physical Chemistry, HU	Dynamics of Photoionization Processes in Biological Molecules
30.4-8.5.06	Prof. P. Devlin, Oklahoma State University	Ice Surface Spectra
11.5.06	Yifat Miller, Fritz Haber Inst. & Dept of Physical Chemistry, HU	Vibrational Spectroscopy and Reaction Dynamics of Atmospheric Molecule
12-20.5.06	Prof. W.M. Gelbart, Chemistry, UCLA	Complex Fluids
17-25.5.06	Prof. B. Honig, Biochem. & Mol. Biophys. Columbia Univ.	Coding Binding Specificity on Protein Surfaces: From Molecules to Cells
	Ayelet Gross, Fritz Haber Center & Dept of Physical Chemistry, HU	Ultra Fast Compression-Induced Processes of Impact-Headed Clusters
	Prof. V. Buch, Fritz Haber Center & Dept of Physical Chemistry, HU	Molecular Crystal Structures from Scratch? And a Quest for HCl Monohydrate Structure
28.6-10.7.06	Dr. J. Lundell, Chemistry, University of Helsinki	Computer Assisted Methods
6.7.06	Mr. M. Rajuan, FH Center & Dept of Physical Chemistry, HU	Molecular Dynamics for Indirect Chemical Reactions – The Kinetic Propagator
4-10.9.06	Prof. U. Buck, MPI Göttingen, Germany	Cluster Dynamics

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4-10.9.06	Dr. B. Abel, Physical & Chemical Graduate School, Göttingen, Germany	Biomolecular Model Systems
17-19.9.06	Quantum Thermodynamic Workshop, Zefat; Prof. R. Kosloff Organizer	R. Kosloff, Hebrew University: Introduction to Quantum Thermodynamics. D. Tannor, Weizmann Institute: Thermodynamic Analysis of Laser Cooling: A Theory of Purity Increasing Transformations. Y. Rezek, Hebrew University: Reciprocating Quantum Heat Engines and Refrigerators. I. Averbuck, Weizmann Institute: Cooling in an Optical Shaker. M. Vilenky, Weizmann Institute: Laser Cooling in a Bistable Cavity. E. Boukobza, Weizmann Institute: Thermodynamics of Light-Matter Interactions. M. Khasin, Hebrew University: Optimal Partition of a Composite System. Z. Amitay, Technion, Haifa: Coherent Control of Multiphoton Excitation Channels and Information. S. Kalush, Hebrew University: The Quantum Governor. E. Frishman, Weizmann Institute: Local Control of Quantum Computation. S. Harel, Hebrew University: Radiation Scattering from Manifolds. Y. Goldfarb, Weizmann Institute: Complex Bohmian. Y. Weinstein, Technion, Haifa: Algorithmic Cooling of Spins.
4-11.9.06	Dr. Ch. Koch, Freie Universität, Berlin	Cold Molecule Formation
2.11.06	Prof. A. Libchaber, Rockefeller University	Physical Aspects of the Origin of Life Problem
16.11.06	Dr. V.A. Parsegian, Physical & Structural Biology Lab, NIH	Van der Waals Forces: Cosmic to Cosmetic
23.11.06	Dr. Masha Niv, Weill Medical College, Cornell University	Computational Insights into Molecular Mechanisms of Cell Signaling
30.11.06	Dr. A. Veksler, Chemical Physics, Weizmann Institute	Phase Separation and Membrane Protrusions Driven by Actin Polymerization and Adhesion
14.12.06	Dr. Dan T. Major, Dept of Chemistry, University of Minnesota	Transition State Stabilization, Carbon α -Proton Acidity, and Nuclear Quantum Mechanical Effects in Enzyme Catalysis
21.12.06	Dr. A. Priel, Dept of Physics, University of Alberta, Edmonton, Canada	Sub-cellular Biological Networks: Electrodynamics Properties of the Cytoskeleton
28.12.06	Dr. O. Farago, Biomedical Engineering BGU, Beer-Sheva	Meso-Scale Computer Modeling of Lipid-DNA complexes for gene therapy
4.1.07	Dr. V. Averbukh, Theoretical Chemistry, University of Heidelberg	Recent Advances in the Study of Interatomic Decay in Clusters
8.1.07	Dr. D. Segal, Dept of Chemistry, Columbia University	Non Equilibrium Dynamics in Spin-Bath Models
11.1.07	Dr. J. Shifman, Inst. of Life Sciences, HU	Design of Protein-Protein Interfaces
15.1.-15.3.07	Dr. A. Adesokan, UC Irvine	
18.1.07	Prof. Z. Amitay, Technion, Haifa	Multiphoton Coherent Control and Information Processing
22-26.1.07	Prof. B. Honig, Chem. & Biochem. Columbia University, New York	
25.1.07	Dr. O. Hod, Dept of Chemistry, Rice University, Houston, USA	Graphene Nanoribbons: New Players in the Field of Nanoelectronics
29.1.07	Dr. M. Nest, Theoretical Chemistry, University of Potsdam	Correlation Quantum Dynamics of Electrons with Multi-Configurational Wave Functions

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List of Visitors and Seminars 2004-2009

1.2.07	Ms. S. Yacoby, Physical Chemistry, HU	Auxiliary and Effective Fields in Molecular Electronic Structure
22-23.2.07	Prof. R. Hernandez, Georgia Inst. of Technology	
25-26.2.07	Prof. L. Tolbert, Georgia Inst. of Technology	
11-14.3.07	Prof. D. Leitner, Cornell University	
10.4.07	Joseph E. Subotnik, Dept of Chemistry, UC Berkeley	Local Correlation Theory: Smooth New Tricks for a Rough Problem
19.4.07	Dr. A. Heidenreich, School of Chemistry, Tel-Aviv University	Extreme Ionization of Clusters by Ultraintense Laser Pulses
26.4.07	Y. Kurzweil, Inst. of Chemistry & FH, HU	Quantum Memory Effects in Electron Dynamics in Metal Clusters
2.5.07	A. Cohen, Inst. of Chemistry & FH, HU	Ultrafast Dynamics of Electronic States in Rare-Gas Matrix Photochemistry
3.5.07	Dr. R. Zangi, Dept of Chemistry, Columbia University, NY	When Hydrophobes Meet Electrolytes: Insights from Computer Experiments
7-13.5.07	Prof. D.J. Tobias, Dept of Chemistry, UC Irvine, CA	Ions at the Air-Water and Membrane-Water Interfaces
14.5.07	Prof. Steven D. Schwartz, Biophys. & Biochem. Seaver Foundation Center for Bioinformatics, Albert Einstein College of Medicine, NY	How Enzymes Catalyze Reactions in Atomic Detail
17.5.07	Prof. R. Benny Gerber, Physical Chemistry & FH, HU	Vibrational States of Biological Molecules: Spectroscopy, Dynamics, and Potential Surfaces
20-28.5.07	Prof. P. Devlin, Oklahoma State University	
29.5-1.6.07	Prof. B. Abel, University of Göttingen	
29.5-1.6.07	Dr. E. Vöhringer-Martinez, University of Göttingen	
31.5.07	Ester Livshits, Physical Chemistry & FH, HU	A Well-Tempered Density Functional Theory of Electrons in Molecules
5-10.6.07	Prof. Mark S. Gordon, Iowa State University and Ames Laboratory	A General Approach to Intermolecular Interactions
5-10.6.07	Dr. B. Njagic, Iowa State University and Ames Laboratory	
17.6-1.7.07	Prof. S. Adhikari, Physical Chem., Indian Assoc. for Cultivation of Science, Jadavpur, Kolkata, India	Beyond Born Oppenheimer: New Approach for Conical Intersections
19-24.6.07	Dr. M. Nest, Potsdam University, Germany	
21.6.07	Dr. Tom Young, Columbia University, NY	The Role of Active Site Water in Protein Ligand Binding
23.6-	Dr. J. Sadlej, University of War-	

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1.8.07	saw	
23.6-1.8.07	Dr. N. Uras-Aytemiz, Suleyman Demirel University, Turkey	
5.7.07	Dr. V.B. Teif, Belarus National Acad. Of Sciences	
5.7.07	Dr. A. Dell Hammerich, Chemistry Dept., Univ. of Illinois Chicago	Defining and Characterizing Dynamic Hydrogen Bonds: An Ab Initio Molecular Dynamics Study of Aqueous Acidic Solutions and Water
24.8-16.9.07	Prof. P. Salamon, San Diego State University	
26.8-31.8.07	Safed Workshop on Cooling and Thermodynamics of Quantum Systems. Organized by Ronnie Kosloff (FH), David Tannor (WIS), and T. Mor (TECHNION).	Alicki, R. Inst. of Theoretical Physics & Astrophysics University of Gdansk, Poland ; Tannor, D. Weizmann Institute, Rehovot; Dr. Mor, T. Computer Science Dept, Technion, Israel Inst. of Technology, Haifa; Andresen, B. Orsted Lab., University of Copenhagen; Boykin, Oscar P., Electrical & Computer Engineering, University of Florida; Diosi, L. Research Inst. for Particle & Nuclear Physics, Budapest; Garcia-Ripoll, J.J, Dpto. De Fisica Teorica, Facultad de CC. Fisicas, Ciudad Universitaria s/n, Madrid 28040, Spain, Universidad Complutense de Madrid; Henrich, Markus, Inst. for Theoretical Physics, University of Stuttgart; Fernandez, J.M.; Kowalewski, Markus, Dept of Chemistry LMU Munchen ; Ritsch, Helmut , Universitaet Innsbruck, Theoretische Physik, Austria; Roychowdhury, V.P., Dept of Electrical Engineering, UCLA; Salamon, P. (San Diego, CA) Dept of Mathematics, SDSU San Diego, CA 92182; Amitay, Z., Dept of Chemistry, Technion; Averbukh, I. Weizmann Institute of Science Rehovoth; Davidson N. Weizmann Institute of Science Rehovoth; Feldmann T, Fritz Haber Center The Hebrew University of Jerusalem; Kurizki G. Weizmann Institute of Science Rehovoth; Nitzan A., School of Chemistry, Tel Aviv University; Boukobza, E. Weizmann Institute of Science Rehovoth; Elias Y. Chemistry, Technion ; Weinstein Y. Chemistry, Technion
2-8.9.07	Safed Workshop on Density Functional Theory. Organized by Leeor Kronik (Weizmann), Roi Baer (FH/HUJI) and E. Rabani (Tel Aviv Univ).	
6-8.9.07	Prof. R. Car, Princeton University	
6-9.9.07	Prof. M. Head-Gordon, UC Berkeley	
23.9-6.10.07	Dr. Ch. Koch, Freie Universität Berlin	
1.11.07	Prof. M. Baer, FH, HU Jerusalem	Born-Oppenheimer Coupling Terms as Molecular Fiels
15.11.07	Ms Michael Steinberg, FH, HU Jerusalem	Structural Changes of Cytochrome c in the Gas Phase
29.11.07	Esteban Vöhringer-Martinez, University of Göttingen & Max-Planck Inst for Biophysical Chemistry	Dynamics of Laser Induced Phase Transitions in Water
6.12.07	Dr. Lukasz Cwiklik, Inst of Chem. & FH Center, HU Jerusalem	Segregation of Inorganic Ions at Surfaces of Polar Nonqueous Liquids
13.12.07	Dr. O. Gat, Racah Inst. of Phys-	Rabi Oscillations on Energy Surfaces: Integr-

	ics, HU	able Phase-Space Dynamics of Cavity QED
16-21.12.07	<p>Minerva Gentner Symposium on Time dependent DFT, Quuen of Sheba Eilat Israel. Organizers: Israel:</p> <p style="padding-left: 40px;">R. Baer (FH/HUJI), E. Rabani (Tel Aviv) L. Kronik (WIS)</p> <p>Germany:</p> <p style="padding-left: 40px;">E. K. U. Gross (Berlin) A. Goerling (Munchen)</p>	<p>Adhikari Satrajit, Indian Association for the Cultivation of Science, Kolkata, India; Argaman Nathan, NRCN, Beer Sheva, Israel; Armiento Rickard, Universitaet Bayreuth, Germany; Baer Michael, The Hebrew University of Jerusalem, Israel; Baer Roi, The Hebrew University of Jerusalem, Israel ; Band Yehuda, Ben Gurion University, Beer Sheva, Israel; Bauer Dieter, Max Planck Institute for Nuclear Physics, Heidelberg, Germany; Bonacic-Koutecky Vlasta, Humboldt-Universitat zu Berlin, Germany; Buchman Omri, Hebrew University of Jerusalem, Israel; Burke Kieron, University of California, Irvine, USA; Casida Mark, Universite Joseph Fourier (Grenoble I), France; Castro Alberto, Free University of Berlin, Germany; Di Ventra Massimiliano, UCSD, La Jolla, California, USA; Dubnikova Faina, The Hebrew University of Jerusalem, Israel; Dunietz Barry D., University Of Michigan, Ann Arbor, USA; Eisenberg Helen, The Hebrew University of Jerusalem, Israel; Evers Ferdinand, Forschungszentrum Karlsruhe, Eggenstein-Leopoldshafen, Germany; Garcia-Lastra Juan Maria, Universidad del Pais Vasco, Colindres, Spain; Gershon Tamar, Hebrew University of Jerusalem, Israel; Goerling Andreas, Universitaet Erlangen-Nuernberg, Erlangen, Germany; Granot Rebecca, The Hebrew University of Jerusalem, Israel; Grimme Stefan, University of Muenster, Germany; Gross Hardy, Free University Berlin, Germany; Hod Oded, Rice University, Huston, Texas, USA; Huang Patrick, Larence Livermore National Laboratory, Livermore, California, USA; Katz Gil, The Hebrew University of Jerusalem, Israel; Kosloff Ronnie, The Hebrew University of Jerusalem, Israel; Kraisler Eli, Tel Aviv University, Israel; Kronik Leeor, Weizmann Institute of Science, Rehovot, Israel; Krylov Anna, USC, Los Angeles, California, USA; Kuemmel Stephan, University of Bayreuth, Germany; Kurth Stefan, Freie Universitaet Berlin, Germany; Kurzweil Yair, University of California Berkeley, USA; Levy Ohad, NRCN, Israel; Livshits Ester, The Hebrew University of Jerusalem, Israel; Makmal Adi, Weizmann Institute of Science, Rehovot, Israel; Makov Guy, NRCN, Israel; Meir Yigal, Ben Gurion University, Beer Sheva, Israel; Mukhopadhyay Debasis, University of Calcuta, India; Mundt Michael, Weizmann Institute of Science, Israel; Myohanen Petri, University of Jyvaskyla, Finland; Natan Amir, Weizmann Institute of Science, Rehovot, Israel; Naveh Doron, Weizmann Institute of Science, Rehovot, Israel; Neuhauser Daniel, UCLA, Los Angeles, California, USA; Niehaus Thomas A., Bremen Center for Computational Science, Germany; Nitzan Abraham, Tel Aviv University, Israel; Pehlke Eckhard, University of Kiel, Germany; Prezhdo Oleg, University of Washington, Seattle, Washington, USA; Rabani Eran, Tel Aviv University, Israel; Rasanen Esa, Freie Universitaet Berlin, Germany; Reinhard Paul-Gerhard, Universitaet Erlangen/Nuernberg, Germany; Rejec Tomaz, Jozef Stefan Institute, Ljubljana, Slovenia; Rom Naomi, Rafael, Haifa, Israel; Ruggenthaler Michael, Max-Planck-Institute for Nuclear Physics, Heidelberg, Germany; Saalfrank Peter, University of Potsdam, Germany; Salzner Ulrike, Bilkent University, Ankara, Turkey; Savin Andreas, CNRS and Universite Pierre et Marie Curie, Paris, France; Schirmer Jochen, University of Heidelberg, Germany; Subotnik Joseph, Tel Aviv University, Israel; Tannor David, Weizmann Institute of Science, Rehovot, Israel; Thiele Mark, Universitaet Bayreuth, Germany; Ullrich Carsten, University of Missouri, Columbia, Missouri, USA; van Leeuwen Robert, University of Jyvaskyla, Finland; Vignale Giovanni, University of Missouri-Columbia, USA; Wang Yong, Bremen Center for Computational Materials Science, Germany; Yabana Kazuhito, University of Tsukuba, Japan; Yang Weitao, Duke University, Durham, North Carolina, USA</p>

Part IV: Appendices
List of Visitors and Seminars 2004-2009

24.12.07	Prof. A. Krylov, Chemistry Dept., USC, LA	Adventures in Fock Space: Dyson Orbitals, Charge Transfer and Properties of Open-Shell Systems
3.1.08	Dr. R. Rohs, Columbia University, NY	The Role of DNA Structure in Protein-DNA Recognition
7.1.08	Prof. S. Malin, Colgate University, Hamilton, NY	What Are Wave Functions?
24.1.08	O. Markovitch, Inst of Chemistry & FH Center HU	Who Moved My Proton?
4.2.08	Prof. B. Abel, University of Göttinge & Max Planck Inst. for Biophysical Chemistry	Dynamics & Applications of Soft Liquid Beam Desorption of Biomolecules with a Laser
7.2.08	Dr. O. Furman, Dept of Molecular Genetics & Biotechnology, Hadassa Medical School, HU	Exploring the Energy Landscape of Protein-Protein Binding with Rosetta
14.2.08	D. Steinitz, Inst of Chemistry & FH Center (HU)	Crystal Reflection – A New Kind of Interferometer for Atoms
18.2.08	Prof. J. Manz, Inst. for Chemistry & Biochem., Freie Universität, Berlin	Wavepacket Dynamics Driven by Laser Pulses
21.2.08	Prof. T. Seideman, Dept of Chemistry, Northwestern University	New Directions in Laser Alignment. From High Harmonic Generation to Guided Molecular Assembly
3.4.08	M. Khasin, Inst. of Chemistry HU (Ph.D. Lecture)	Efficient Simulation of Quantum Evolution Using Dynamics Coarse-Graining
10.4.08	Prof. R. Podgornik, Inst. Jozef Stefan, Ljubljana, Slovenia	Quenched Disorder and Coulomb Interactions
14.4.08	Prof. Zhigang Shuai, Chinese Academy of Sciences, Beijing	Carrier Transports in Organic Semiconductors: Band vs. Hopping Descriptions
15.5.08	M. Assaf, Racah Inst. of Physics, HU	Noise Enhanced Persistence in Biochemical Regulator Networks with Feedback Control
18-22.5.08	1st International Symposium on Improvised Explosives, Rosh Hanikra	
22.5.08	Prof. P. Jungwirth, Acad. of Sciences, Czech Republic, Prague	Ions at Aqueous Interfaces: From Water Surface to Hydrated Proteins
26.5.08	Prof. E. Geva, Dept of Chem. & FOCUS Center, Univ. of Michigan, Ann Arbor	Vibrational Energy Relaxation and Multi-Dimensional Infrared Spectroscopy of a Vibrational Mode Strongly Coupled to its Environment
3-4.6.08	Conference in Honor of ABS's Birthday –Mishkenot Shaananim	
16.6.08	Prof. B. Dunietz, Dept of Chem., University of Michigan, Ann Arbor	Exploring Conductance Switching Properties of Molecular and Nano-Scale Devices – A Computational Approach
19.6.08	Prof. P. Brumer, Dept of Chem., University of Toronto	Laser-Induced Femtosecond Electrical Currents in Molecular Wires: From Fundamentals to Polyacetylene

Part IV: Appendices
List of Visitors and Seminars 2004-2009

24.7.08	Prof. S. Kuemmel, Physics Inst., University of Bayreuth, Germany	Quantum Mechanics Without a Wavefunction: Problems and Prospects in Density Functional Theory
31.7.08	Prof. B. Tsukerblat, Dept of Chem., BGU, Beer Sheva	Nanosopic Cluster V15: Spin Frustration and Antisymmetric Exchange
4.8.08	Dr. L. Kronik, Dept of Materials & Interfaces, Weizmann Inst. of Science	Understanding Electronic Properties at Molecule/Inorganic-Solid Interfaces of First Principles
6.11.08	Professor Ruth M. Lynden-Bell University Chemical Lab., Cambridge, UK	Towards Understanding Water: Simulations of Modified Water Models
10.11.08-14.11.08	Prof. P. Devlin, Oklahoma State Univ.	
10.11.08	Professor Thomas Weinacht Physics Dept, Stony Brook University, NY	Controlling Molecular Dissociation using Strong Laser Fields
12.11.08	Professor Fillipp Furche, University of California, Irvine	Electronic Structure Calculations as a Tool in Chemistry
25.11.08-29.11.08	Professor Vladimir Feldman Moscow State University, Russia	A New Look at Radiation Chemistry of Matrix-Isolated Molecules: Modeling Primary Events in Condensed Phase
2.12.08	Prof. Svatopluk Zeman, Inst of Energetic Materials, University of Pardubice, Czech Republic	Initiation Reactivity of the Individual Polynitro Compounds – Specification of Reaction Center
4.12.08	Prof. Nir Gov, Chemical Physics, Weizmann Inst., Rehovot	Dynamic Instability in an Expanding Cell Culture
6.12.08	Dr. Lukasz Cwiklik, Inst. of Chemistry & FH Center, HU	Segregation of Inorganic Ions at Surfaces of Polar Nonaqueous Liquids
18.12.08	Dr. Michal Sharon, Biological Chemistry, Weizmann Inst. of Science	Weighing the Evidence for Structure: Mass Spectrometry of the Degradation Machinery
13.1.09	Prof. David J. Srolovitz, Yeshiva College, NY	Why Do ZnO Nanoribbons Spontaneously Bend?
29.1.09	Dr. Emmanuel Tannenbaum, Chemistry Dept., BGU, Beer-Sheva	Diploidy, Homologous Recombination Repair, and the Selective Advantage for Secual Reproduction in Unicellular Organisms
4.2.09	Prof. Igal Szleifer, Dept of Biol. & Chem. Eng., Northwestern U., Chicago	Thermodynamics and Kinetics of Protein Adsorption
13.2.09-19.2.09	Prof. J. Manz, Inst. for Chemistry & Biochem., Freie Universität, Berlin	
9.3.09	Dr. Arik Landau, Chemistry Dept., USC	The Frozen Natural Orbital (FNO) Equation-of-Motion Coupled-Cluster (EOM-CC) Approach

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List of Visitors and Seminars 2004-2009

15.3.09-29.3.09	Dr. Christiane Koch, Free Univ. Berlin	
21.3.09-29.3.09	Dr. Mamadou Ndong, Free Univ. Berlin	
16.3.09	Dr. Oleg S. Vasyutinskii, Ioffe Inst., Russian Acad. of Sci., St. Petersburg	Orbital Polarization of the Chemical Reaction Products: Experimental Determination of the Dynamical Amplitudes and Phases
26.3.09	Prof. Stephen Leone, Dept of Chemistry, UC Berkeley	X-Ray Probing of Atomic and Molecular Dynamics to the Attosecond Limit
31.3.09	Prof. Martin Zanni, Dept of Chemistry, Univ. of Wisconsin, Madison	2-D IR Spectroscopy and Isotope Labeling Defines the Pathway of Amyloid Formation with Residue Specific Resolution
23.4.09	Dr. Mary K. Gilles, Lawrence Berkeley National Lab., Berkeley, CA	Probing Atmospheric Aerosols by Micro-Spectroscopic Methods
30.4.09	Fritz Haber & Farkas Centers	Dr. Baruch Barzel Racah Inst. of Physics, HU
30.4.09	Dr. Baruch Barzel Racah Inst. of Physics, HU	A Simple Simulation for a Complex Network
5.5.09-19.5.09	Prof. Brian Burrows, Staffordshire University	
10.5.09	Prof. Pavel Jungwirth Inst of Organic Chem & Biochem, Acad. Sci. Czech Republic	Calculations of Photoionization in Water: Electrons, Cationic Holes, and Ionized DNA Bases
14.5.09	Dr. Maytal Caspary Toroker Faculty of Chem. & Meitner Center for Computational Quantum Chem., Technion	Flux Correlation Approach to Electronic Transport through Molecular Junctions
25-26.5.09	Symposium on Interfaces At Kibbutz Tzuba	Attendance and participation of the Beirat members
24-29.5.09	Prof. Dr. W. Domcke, Tech. Univ. Munchen	
24-27.5.09	Prof. Dr. G. Meijer, Fritz Haber Institute, Berlin	
24-27.5.09	Prof. Dr. H. Grubmüller, Max-Planck-Institut für biophysikalische Chemie	
26.5.09-1.6.09	Prof. P. Devlin, Oklahoma State Univ.	
11.6.09	Dr. Yoav Tsori Dept of Chem. Eng. BG University of The Negev	Phase Separation Transition in Liquids and Polymers in Electric Field Gradients
3.8.09	Prof. Ilan Benjamin Dept of Chemistry, UCSC	Water Structure at Interfaces and Chemical Reactivity
15.10.09	Dr. Jiri Vala Dept of Math. Physics, Nat. University of Ireland	Topological Quantum Computing
19.10.09	Prof. Emily Allyn Weiss Dept of Chemistry, Northwestern University	Chemical Control of the Optical Properties of CdSe QD-Organic Complexes
28.10.09	Prof. Daniel Harries	Driving Macromolecular Self Organization by

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	Inst of Chem. & FH Center HU	Crowding and Osmotic Stress
10.11.09	Prof. David Chandler Dept of Chemistry, UC Berkeley	Sampling Trajectory Space to Study Rare Events and Non-Equilibrium Order - Disorder
30.11.09	Prof. Erik T.J. Nibbering Max-Born-Inst., Berlin	Ultrafast Vibrational Spectroscopy of Bimolecular Reaction Dynamics in Liquid Solution
10.12.09	Computational Chemistry Symposium	<p>J. Sauer (Humboldt University, Berlin): C-H activation by transition metal oxides – from gas phase clusters to supported catalysts</p> <p>D. Danovich (HU): No-pair bonding in the high spin states of metal clusters</p> <p>T. Ansbacher (HU): Copper-Keepers – copper chaperones and their coordination number of Cu(I)</p> <p>W.L. Jorgensen (Yale University): From water models to drug lead optimization</p> <p>M. Amity (HU): Hydrolysis of organophosphate compounds by mutant Butyrylcholinesterase – A story of two histidines]</p> <p>R. Politi (HU): Osmolytes modulate peptide folding</p> <p>A. Dreuw (J.W. Goethe University, Frankfurt): Photo-initiated processes in the medium-sized organic pigments</p> <p>T. Stein (HU): Charge transfer excitations using Time-Dependent Density Functional Theory</p> <p>P. Schyman (HU): Brain chemistry: How does P450 catalyze the formation of neurotransmitters</p> <p>S. Amaran (HU): The photoassociation of Mg₂</p> <p>E.F. Sheka (Friendship University of the Russian Federation, Moscow): Fullerene-cluster amplifiers and nanophotonics of fullerene solutions</p> <p>L. Pele (HU): Anharmonic vibrational spectroscopy calculations for biological molecules: new algorithms and applications</p> <p>Ch. Dryzun (HU): Novel general symmetry measures</p>
24.12.09	Prof. David J. Tannor Weizmann Institute, Rehovot	How Did Pauli Miss It: An Exact Formulation of Quantum Mechanics with Complex Trajectories

LIST OF PUBLICATIONS 2004-2009

NOAM AGMON

114. A.V. Popov, N. Agmon, I.V. Gopich and A. Szabo Influence of Diffusion on the Kinetics of Excited-State Association-Dissociation Reactions: Comparison of Theory and Simulation, *J. Chem. Phys.* 120, 6111-6116 (2004).
115. S.-H. Park, K.-J. Shin and N. Agmon, Exact Solution of the Excited-State Geminate $A^*BC^* + D$ Reaction with Two Different Lifetimes and Quenching, *J. Chem. Phys.* 121, 868-876 (2004).
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117. H. Lapid, N. Agmon, M.-K. Petersen and G.A. Voth, A Bond-Order Analysis of the Mechanism for Hydrated Proton Mobility in Liquid Water, *J. Chem. Phys.* 122, (2005).
118. N. Agmon, Elementary Steps in Excited-State Proton Transfer, *J. Phys. Chem. A* 109, 13-35 (2005).
119. N. Agmon, Proton Pathways in Green Fluorescence Protein, *Biophys. J.* 88, 2452-2461 (2005).
120. D. Dantsker, U. Samuni, J.M. Friedman and N. Agmon, A Hierarchy of Functionally Importance Relaxations within Myoglobin Based on Solvent Effects, Mutations and Kinetic Model, *Biochim. Biophys. Acta: and Proteomics* 1749, 234-251 (2005).
121. S. Park, K.J. Shin, A.V. Popov and N. Agmon Diffusion-Influenced Excited-State Reversible Transfer Reactions, $A^*+B=C^*+D$, with Two Different Lifetimes: Theories and Simulation, *J. Chem. Phys.* 123, 034507 (2005).
122. P. Leiderman, D. Huppert and N. Agmon, Transition in the Temperature Dependence of GFP Fluorescence: From Proton Wires to Proton Exit, *Biophys. J.* 90, 1009-1018 (2006).
123. N. Agmon, Reduced Parameter Set Determinable from Geminate Kinetics, *Chem. Phys. Lett.* 417, 530-534 (2006).
124. R. Gepshtein, D. Huppert and N. Agmon Deactivation Mechanism of the Green Fluorescent Chromophore, *J. Phys. Chem. B* 110, 4434-4442 (2006).
125. N. Agmon, Kinetics of switchable proton escape from a proton-wire within green fluorescence protein, *J. Phys. Chem. B* 111, 7870 (2007).
126. O. Markovitch and N. Agmon, Structure and energetics of the hydronium hydration shells, *J. Phys. Chem. A* 111, 2253 (2007).
127. N. Agmon, "Kinetics of switchable proton escape from a proton-wire within green fluorescence protein", *J. Phys. Chem. B* 111, 7870-7878 (2007).
128. O. Markovitch and N. Agmon, "Structure and energetics of the hydronium hydration shells", *J. Phys. Chem. A* 111, 2253-2256 (2007).
129. O. Markovitch and N. Agmon, "The distribution of acceptor and donor hydrogen-bonds in bulk liquid water", *Mol. Phys.* 106, 485-495 (2008).
130. O. Markovitch and N. Agmon, "Reversible geminate recombination of hydrogen-bonded water molecule pair", *J. Chem. Phys.* 129, 084505 (2008).
131. O. Markovitch, H. Chen, S. Izvekov, F. Paesani, G. A. Voth, and N. Agmon, "Special pair dance and partner selection: Elementary steps in proton transport in liquid water", *J. Phys. Chem. B* 112, 9456-9466 (2008).
132. S. Park and N. Agmon, "Concentration profiles near an activated enzyme", *J. Phys. Chem. B* 112, 12104-12114 (2008).
133. S. Park and N. Agmon, "Theory and simulation of diffusion-controlled Michaelis-Menten kinetics for a static enzyme in solution", *J. Phys. Chem. B* 112, 5977-5987 (2008).
134. S. Park and N. Agmon, "Multisite reversible geminate reaction", *J. Chem. Phys.* 130, 074507 (2009).
135. A. Shinobu and N. Agmon, "Mapping Proton Wires in Proteins: Carbonic Anhydrase and GFP Chromophore Biosynthesis", *J. Phys. Chem. A* 113, 7253-7266 (2009).
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78. G. J. Halasz, A. Vibok, R. Baer, and M. Baer, Conical intersections induced by the Renner effect in polyatomic molecules, *Journal of Physics a-Mathematical and Theoretical* 40, F267 (2007).

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based on Aharonov-Bohm interferometry, *J. Phys. C* 20, 383201 (2008).

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90. T. Stein, L. Kronik, and R. Baer, Reliable Prediction of Charge Transfer Excitations in Molecular Complexes Using Time-Dependent Density Functional Theory, *J. Am. Chem. Soc.* 131, 2818 (2009).

91. H. R. Eisenberg and R. Baer, "A new generalized Kohn-Sham method for fundamental band-gaps in solids", *Phys. Chem. Chem. Phys.* 11, 4674-4680 (2009).

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Transition from Lamellipodium to Filopodium in a Membrane Free System" *Proc. Nat'l Acad. Sci. USA* 103, 4906-4911 (2006).

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