



Roi Baer: Curriculum Vitae (December 16, 2021)

The Ratner Family Chair in Chemistry, Fritz Haber Research Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel. (roi.baer@huji.ac.il)

Academic Education

- 1982 Hebrew University of Jerusalem, B.Sc. Mathematics and Physics
- 1993 Hebrew University of Jerusalem, M.Sc. Chemistry
- 1996 Hebrew University of Jerusalem, Ph.D. Chemistry
- 1998 University of California, Berkeley (Postdoc)

Faculty Positions

- 1998 Hebrew University of Jerusalem, Senior lecturer of Theoretical Chemistry
- 2002 Hebrew University of Jerusalem, Associate Professor of Theoretical Chemistry
- 2006 Hebrew University of Jerusalem, Professor of Theoretical Chemistry

Academic Positions

- 2005-6 University of California at Los Angeles, Visiting Professor
- 2006-7 Hebrew University of Jerusalem, Chair, Dept. of Physical Chemistry
- 2006- Hebrew University of Jerusalem, Director of the Fritz Haber Research Center
- 2008 University of Southern California at Los Angeles, Visiting Professor
- 2011-15 Hebrew University of Jerusalem, Co-director of the Hoffman Leadership and Responsibility Program
- 2015-16 University of California Berkeley, Visiting Pitzer Professor
- 2015-16 Heising-Simons Visiting Fellow of the Kavli Energy Nanoscience Institute at UC Berkeley

Editorial/Advisory Boards

- 2003 Invited Editor of Special Issue on Computational Chemistry; Israel Journal of Chemistry
- 2006-7 Editorial Advisory Board "Physical Chemistry-Chemical Physics"
- 2008-11 Member of the Fellowships Committee of Minerva Steiftung in the Max Planck Society
- 2010-14 Member of Editorial Committee of Annual Reviews of Physical Chemistry
- 2011 Voted chair of 2015 Gordon Conference on Time Dependent Density Functional Theory
- 2011 Chemical Physics, Guest co-Editor for Special Issue, *Open Problems in TDDFT*
- 2011-12 Associate Editor of Theoretical Chemistry Accounts (Springer)
- 2013-15 Member of JPC Editorial Advisory Board

Student and postdoc mentoring

Postdoc	Dr. Yair Kurzweil, Dr. Ester Livshits, Dr. Helen Eisenberg, Dr. Zhu Ruan
Ph.D.	Dr. Shlomit Jacoby, Dr. Rebecca Granot, Dr. Ester Livshits, Dr. Oded Hod, Dr. Tamar Stein, Dr. Adva Baratz, Dr. Vojtech Vlcek, Dr. Omri Buchman, Dr. Marcel Fabian, Dr. Yael Cytter, Dr. Eitam Arnon, Ben Shpiro, Rebecca Hadad, Stanislav Zelner, Sayak Adhikari
M. Sc.	Dr. Itai Ryb, Nadal Siam, Muhammad Attrash, Dr. Yael Cytter, Dr. Rebecca Hadad, Sayak Adhikari

Teaching

Introduction to Chemical Bonding
Theoretical Methods and Techniques in Chemistry
Physical Chemistry III
Density Functional Theory
Advanced Laboratory in Chemical Physics

Honors and Awards

1995	Wolf Foundation prize for Ph.D. students
1996	The Fritz Haber research center prize
2000	The Josepha and Leonid Olschwang prize, Israel Academy of Science
2001	Noted “Excellent Teacher” of the Science Faculty
2007	Noted “Excellent Teacher” of the Science Faculty
2013	The Klachky Prize for the Advancement of the Frontiers of Science
2015	The Ratner Family Chair in Chemistry
2018	Hebrew University Rector’s Prize for Excellence in Research and Teaching

Publications

- [1] Minh Nguyen, Wenfei Li, Barry (Yangtao) Li, Roi Baer, Eran Rabani, and Daniel Neuhauser. Tempering stochastic density functional theory. *J. Chem. Phys.*, page 5.0063266, October 2021.
- [2] Marcel David Fabian, Ben Shpiro, and Roi Baer. Linear scalability of density functional theory calculations without imposing electron localization. *arXiv:2108.13478 [physics]*, August 2021. arXiv: 2108.13478.
- [3] Ben Shpiro, Marcel David Fabian, Eran Rabani, and Roi Baer. Forces from stochastic density functional theory under nonorthogonal atom-centered basis sets. *arXiv:2108.06770 [physics]*, August 2021. arXiv: 2108.06770.
- [4] Krishnendu Gope, Ester Livshits, Dror M. Bittner, Roi Baer, and Daniel Strasser. Two pathways and an isotope effect in H₃⁺ formation following double ionization of methanol. *Natural Sciences*, page ntl.10022, July 2021.
- [5] Ming Chen, Roi Baer, Daniel Neuhauser, and Eran Rabani. Stochastic density functional theory: Real- and energy-space fragmentation for noise reduction. *J. Chem. Phys.*, 154(20):204108, May 2021.

- [6] Vladimir U. Nazarov and Roi Baer. The high frequency limit of spectroscopy. *arXiv:2101.09467 [cond-mat]*, January 2021. arXiv: 2101.09467.
- [7] Nadine C. Bradbury, Chern Chuang, Arundhati P. Deshmukh, Eran Rabani, Roi Baer, Justin R. Caram, and Daniel Neuhauser. Stochastically Realized Observables for Excitonic Molecular Aggregates. *J. Phys. Chem. A*, 124(49):10111–10120, December 2020.
- [8] Eitam Arnon, Eran Rabani, Daniel Neuhauser, and Roi Baer. Efficient Langevin dynamics for “noisy” forces. *J. Chem. Phys.*, 152(16):161103, April 2020.
- [9] Ester Livshits, Itamar Luzon, Krishnendu Gope, Roi Baer, and Daniel Strasser. Time-resolving the ultrafast H₂ roaming chemistry and H₃⁺ formation using extreme-ultraviolet pulses. *Communications Chemistry*, 3(1):49, December 2020.
- [10] Wenjie Dou, Ming Chen, Tyler Y. Takeshita, Roi Baer, Daniel Neuhauser, and Eran Rabani. Range-separated stochastic resolution of identity: Formulation and application to second-order Green’s function theory. *J. Chem. Phys.*, 153(7):074113, August 2020.
- [11] Alex J. Lee, Ming Chen, Wenfei Li, Daniel Neuhauser, Roi Baer, and Eran Rabani. Dopant levels in large nanocrystals using stochastic optimally tuned range-separated hybrid density functional theory. *Phys. Rev. B*, 102(3):035112, July 2020.
- [12] Xu Zhang, Gang Lu, Roi Baer, Eran Rabani, and Daniel Neuhauser. Linear-Response Time-Dependent Density Functional Theory with Stochastic Range-Separated Hybrids. *J. Chem. Theory Comput.*, 16(2):1064–1072, February 2020.
- [13] Krishnendu Gope, Ester Livshits, Dror M. Bittner, Roi Baer, and Daniel Strasser. Absence of Triplets in Single-Photon Double Ionization of Methanol. *The Journal of Physical Chemistry Letters*, 11(19):8108–8113, October 2020.
- [14] Ming Chen, Roi Baer, Daniel Neuhauser, and Eran Rabani. Energy window stochastic density functional theory. *J. Chem. Phys.*, 151(11):114116, September 2019.
- [15] Ming Chen, Roi Baer, Daniel Neuhauser, and Eran Rabani. Overlapped embedded fragment stochastic density functional theory for covalently-bonded materials. *J. Chem. Phys.*, 150(3):034106, January 2019.
- [16] Yael Cytter, Eran Rabani, Daniel Neuhauser, Martin Preising, Ronald Redmer, and Roi Baer. Transition to metallization in warm dense helium-hydrogen mixtures using stochastic density functional theory within the Kubo-Greenwood formalism. *Physical Review B*, 100(19), November 2019.
- [17] Wenjie Dou, Tyler Y. Takeshita, Ming Chen, Roi Baer, Daniel Neuhauser, and Eran Rabani. Stochastic Resolution of Identity for Real-Time Second-Order Green’s Function: Ionization Potential and Quasi-Particle Spectrum. *J. Chem. Theory Comput.*, October 2019.
- [18] Marcel D. Fabian, Ben Shpiro, Eran Rabani, Daniel Neuhauser, and Roi Baer. Stochastic density functional theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 10.1002/wcms.1412(0):e1412, 2019.
- [19] Tufan Ghosh, Joanna Dehnel, Marcel Fabian, Efrat Lifshitz, Roi Baer, and Sanford Ruhman. Spin Blockades to Relaxation of Hot Multiexcitons in Nanocrystals. *J. Phys. Chem. Lett.*, 10(10):2341–2348, May 2019.
- [20] Wenfei Li, Ming Chen, Eran Rabani, Roi Baer, and Daniel Neuhauser. Stochastic embedding DFT: Theory and application to p-nitroaniline in water. *J. Chem. Phys.*, 151(17):174115, November 2019.

- [21] Itamar Luzon, Ester Livshits, Krishnendu Gope, Roi Baer, and Daniel Strasser. Making Sense of Coulomb Explosion Imaging. *J. Phys. Chem. Lett.*, 10(6):1361–1367, March 2019.
- [22] Egor Ospadov, Stuart M. Rothstein, and Roi Baer. Quantum Monte Carlo assessment of density functionals for π -electron molecules: ethylene and bifuran. *Molecular Physics*, 117(17):2241–2250, September 2019.
- [23] Vojtěch Vlček, Roi Baer, and Daniel Neuhauser. Stochastic time-dependent DFT with optimally tuned range-separated hybrids: Application to excitonic effects in large phosphorene sheets. *J. Chem. Phys.*, 150(18):184118, May 2019.
- [24] Vojtěch Vlček, Eran Rabani, Roi Baer, and Daniel Neuhauser. Nonmonotonic band gap evolution in bent phosphorene nanosheets. *Phys. Rev. Materials*, 3(6):064601, June 2019.
- [25] Roi Baer and Leeor Kronik. Time-dependent generalized Kohn–Sham theory. *The European Physical Journal B*, 91(7), July 2018.
- [26] Yael Cytter, Eran Rabani, Daniel Neuhauser, and Roi Baer. Stochastic Density Functional Theory at Finite Temperatures. *Phys. Rev. B*, 97:115207, 2018.
- [27] Samuel Hernandez, Yantao Xia, Vojtěch Vlček, Robert Boutelle, Roi Baer, Eran Rabani, and Daniel Neuhauser. First-principles spectra of Au nanoparticles: from quantum to classical absorption. *Molecular Physics*, 116(19-20):2506–2511, October 2018.
- [28] Zhu Ruan and Roi Baer. Unravelling open-system quantum dynamics of non-interacting Fermions. *Mol. Phys.*, 116:2490–2496, 2018.
- [29] Vojtěch Vlček, Roi Baer, Eran Rabani, and Daniel Neuhauser. Simple eigenvalue-self-consistent δ GW0. *J. Chem. Phys.*, 149(17):174107, November 2018.
- [30] Vojtěch Vlček, Wenfei Li, Roi Baer, Eran Rabani, and Daniel Neuhauser. Swift G W beyond 10,000 electrons using sparse stochastic compression. *Phys. Rev. B*, 98(7):075107, August 2018.
- [31] Eitam Arnon, Eran Rabani, Daniel Neuhauser, and Roi Baer. Equilibrium configurations of large nanostructures using the embedded saturated-fragments stochastic density functional theory. *The Journal of Chemical Physics*, 146(22):224111, June 2017.
- [32] Omri Buchman and Roi Baer. Stochastic method for calculating the ground-state one-body density matrix of trapped Bose particles in one dimension. *Phys. Rev. A*, 96(3):033626, September 2017.
- [33] Rebecca Efrat Hadad and Roi Baer. Minimally corrected partial atomic charges for non-covalent electrostatic interactions. *Molecular Physics*, 115(24):3155–3163, December 2017.
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- [35] Daniel Neuhauser, Roi Baer, and Dominika Zgid. Stochastic self-consistent second-order Green’s function method for correlation energies of large electronic systems. *J. Chem. Theory Comput.*, 13:5396–5403, 2017.
- [36] Tyler Y. Takeshita, Wibe A. de Jong, Daniel Neuhauser, Roi Baer, and Eran Rabani. Stochastic Formulation of the Resolution of Identity: Application to Second Order Møller–Plesset Perturbation Theory. *J. Chem. Theory Comput.*, 13(0):4605, 2017.
- [37] Vojtěch Vlček, Eran Rabani, Daniel Neuhauser, and Roi Baer. Stochastic GW Calculations for Molecules. *Journal of Chemical Theory and Computation*, 13(10):4997–5003, October 2017.

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- [40] Daniel Neuhauser, Eran Rabani, Yael Cytter, and Roi Baer. Stochastic Optimally Tuned Range-Separated Hybrid Density Functional Theory. *J. Phys. Chem. A*, 120(19):3071–3078, May 2016.
- [41] Vojtěch Vlček, Helen R. Eisenberg, Gerd Steinle-Neumann, Daniel Neuhauser, Eran Rabani, and Roi Baer. Spontaneous Charge Carrier Localization in Extended One-Dimensional Systems. *Physical Review Letters*, 116(18), May 2016.
- [42] Yi Gao, Daniel Neuhauser, Roi Baer, and Eran Rabani. Sublinear scaling for time-dependent stochastic density functional theory. *J. Chem. Phys.*, 142(3):034106, 2015.
- [43] Shlomit Jacobi and Roi Baer. Smoothing and extrapolating shifted-contour auxiliary-field Monte Carlo signals using discrete Laguerre functions. *arXiv preprint arXiv:1504.05452*, 2015.
- [44] Ioannis D Petsalakis, Giannoula Theodorakopoulos, Omri Buchman, and Roi Baer. Applicability of Mulliken’s formula for photoinduced and intramolecular charge-transfer energies. *Chem. Phys. Lett.*, 625:98–103, 2015.
- [45] Eran Rabani, Roi Baer, and Daniel Neuhauser. Time-dependent stochastic Bethe-Salpeter approach. *Phys. Rev. B*, 91(23):235302, 2015.
- [46] Yihan Shao, Zhengting Gan, Evgeny Epifanovsky, Andrew T. B. Gilbert, Michael Wormit, Joerg Kussmann, Adrian W. Lange, Andrew Behn, Jia Deng, Xintian Feng, Debashree Ghosh, Matthew Goldey, Paul R. Horn, Leif D. Jacobson, Ilya Kaliman, Rustam Z. Khaliullin, Tomasz Kus, Arie Landau, Jie Liu, Emil I. Proynov, Young Min Rhee, Ryan M. Richard, Mary A. Rohrdanz, Ryan P. Steele, Eric J. Sundstrom, H. Lee Woodcock III, Paul M. Zimmerman, Dmitry Zuev, Ben Albrecht, Ethan Alguire, Brian Austin, Gregory J. O. Beran, Yves A. Bernard, Eric Berquist, Kai Brandhorst, Ksenia B. Bravaya, Shawn T. Brown, David Casanova, Chun-Min Chang, Yunqing Chen, Siu Hung Chien, Kristina D. Closser, Deborah L. Crittenden, Michael Diedenhofen, Robert A. DiStasio Jr, Hainam Do, Anthony D. Dutoi, Richard G. Edgar, Shervin Fatehi, Laszlo Fusti-Molnar, An Ghysels, Anna Golubeva-Zadorozhnaya, Joseph Gomes, Magnus W. D. Hanson-Heine, Philipp H. P. Harbach, Andreas W. Hauser, Edward G. Hohenstein, Zachary C. Holden, Thomas-C. Jagau, Hyunjun Ji, Benjamin Kaduk, Kirill Khistyayev, Jaehoon Kim, Jihan Kim, Rollin A. King, Phil Klunzinger, Dmytro Kosenkov, Tim Kowalczyk, Caroline M. Krauter, Ka Un Lao, Adele D. Laurent, Keith V. Lawler, Sergey V. Levchenko, Ching Yeh Lin, Fenglai Liu, Ester Livshits, Rohini C. Lochan, Arne Luenser, Prashant Manohar, Samuel F. Manzer, Shan-Ping Mao, Narbe Mardirossian, Aleksandr V. Marenich, Simon A. Maurer, Nicholas J. Mayhall, Eric Neuscamman, C. Melania Oana, Roberto Olivares-Amaya, Darragh P. O’Neill, John A. Parkhill, Trilisa M. Perrine, Roberto Peverati, Alexander Prociuk, Dirk R. Rehn, Edina Rosta, Nicholas J. Russ, Shaama M. Sharada, Sandeep Sharma, David W. Small, Alexander Sodt, Tamar Stein, David Stock, Yu-Chuan Su, Alex J. W. Thom, Takashi Tsuchimochi, Vitalii Vanovschi, Leslie Vogt, Oleg Vydrov, Tao Wang, Mark A. Watson, Jan Wenzel, Alec White, Christopher F. Williams, Jun Yang, Sina Yeganeh, Shane R. Yost, Zhi-Qiang You, Igor Ying Zhang, Xing Zhang, Yan Zhao, Bernard R. Brooks, Garnet K. L. Chan, Daniel M. Chipman, Christopher J. Cramer, William A. Goddard III, Mark S. Gordon, Warren J. Hehre, Andreas Klamt, Henry F. Schaefer III, Michael W. Schmidt, C. David Sherrill, Donald G. Truhlar, Arieh Warshel, Xin Xu, Alan Aspuru-Guzik, Roi Baer, Alexis T. Bell, Nicholas A. Besley, Jeng-Da Chai, Andreas Dreuw, Barry D. Dunietz, Thomas R. Furlani, Steven R. Gwaltney, Chao-Ping Hsu, Yousung Jung, Jing Kong, Daniel S. Lambrecht, WanZhen Liang, Christian Ochsenfeld, Vitaly A. Rassolov, Lyudmila V. Slipchenko, Joseph E.

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- [48] Adva Baratz, Alexander J. White, Michael Galperin, and Roi Baer. Effects of Electromagnetic Coupling on Conductance Switching of a Gated Tunnel Junction. *J. Phys. Chem. Lett.*, 5(20):3545–3550, October 2014.
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- [50] David A Egger, Shira Weissman, Sivan Refaely-Abramson, Sahar Sharifzadeh, Matthias Dauth, Roi Baer, Stephan Kümmel, Jeffrey B Neaton, Egbert Zojer, and Leeor Kronik. Outer-valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. *J. Chem. Theory Comput.*, 10(5):1934–1952, 2014.
- [51] Helen R. Eisenberg and Roi Baer. Exothermic Mechanism for the Abstraction of Hydrogen from Methane on Li-Doped MgO. *J. Phys. Chem. C*, 119(1):196–215, 2014.
- [52] Hagai Eshet, Roi Baer, Daniel Neuhauser, and Eran Rabani. Multiexciton Generation in Seeded Nanorods. *J. Phys. Chem. Lett.*, 5(15):2580–2585, 2014.
- [53] Daniel Neuhauser, Roi Baer, and Eran Rabani. Communication: Embedded fragment stochastic density functional theory. *J. Chem. Phys.*, 141(4):041102, 2014.
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- [58] Adva Baratz, Michael Galperin, and Roi Baer. Gate-Induced Intramolecular Charge Transfer in a Tunnel Junction: A Nonequilibrium Analysis. *J. Phys. Chem. C*, 117(20):10257–10263, May 2013.
- [59] Qinghui Ge, Yi Gao, Roi Baer, Eran Rabani, and Daniel Neuhauser. A Guided Stochastic Energy-Domain Formulation of the Second Order Møller–Plesset Perturbation Theory. *J. Phys. Chem. Lett.*, 5(1):185–189, 2013.
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