האוניברסיטה העברית בירושלים
THE HEBREW UNIVERSITY OF JERUSALEM
الجامعة العبرية في اورشليم القدس

Roi Baer: Curriculum Vitae (July 11, 2024)

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

2005–06	University of California at Los Angeles, Visiting Professor
2006–07	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
2011–19	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
2006–07	Editorial Advisory Board "Physical Chemistry-Chemical Physics"
2008–14	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 Journal Physical Chemistry Editorial Advisory Board

Student and postdoc mentoring

Postdoc	Dr. Yair Kurzweil, Dr. Ester Livshits, Dr. Helen Eisenberg, Dr. Zhu Ruan, Dr. Marcel Fabian, Dr. Prashant Raj
Ph.D.	Dr. Shlomit Jacoby, Dr. Rebecca Granot, Dr. Ester Livshits, Prof. Oded Hod (TAU), Prof. Tamar Stein (HUJI), Dr. Adva Baratz, Prof. Vojtech Vlcek (UC Santa Barbara), Dr. Omri Buchman, Dr. Marcel Fabian, Dr. Yael Cytter, Dr. Eitam Arnon, Dr. Ben Shpiro, Rebecca Hadad, Sayak Adhikari
M. Sc.	Dr. Itai Ryb, Nidal Siam, Dr. Muhammad Attrash, Dr. Yael Cytter, Rebecca Hadad, Sayak Adhikari, Pavel Savchenko, Anat Hornreich

Teaching

Introduction to the Chemical Bond (undergraduate)
Density Functional Theory (graduate)
Theoretical Methods and Techniques in Chemistry (graduate)
Physical Chemistry III (graduate)
Advanced Laboratory in Chemical Physics (under graduate)
Developing e-learning material for quantum mechanics (with Ronnie Kosloff)

Honors and Awards

1995	Wolf Foundation prize
1996	The Fritz Haber research center prize
2000	The Josepha and Leonid Olschwang prize, Israel Academy of Science
2001, 2007, 2011, 2017, 2018, 2022, 2023	Noted "Excellent Teacher" of the Hebrew University
2013	The Klachky Prize for the Advancement of the Frontiers of Science
2015	The Ratner Family Chair in Chemistry
2018	Rector's Prize for Excellence in Research and Teaching

Publications (Roi Baer)

[1] Rebecca Efrat Hadad, Argha Roy, Eran Rabani, Ronald Redmer, and Roi Baer. Stochastic density functional theory combined with Langevin dynamics for warm dense matter. *Phys. Rev. E*, 109(6):065304, June 2024.

[2] Ester Livshits, Dror M. Bittner, Florian Trost, Severin Meister, Hannes Lindenblatt, Rolf Treusch, Krishnendu Gope, Thomas Pfeifer, Roi Baer, Robert Moshammer, and Daniel Strasser. Symmetry-breaking dynamics of a photoionized carbon dioxide dimer. *Nat. Commun*, in press, 2024.

[3] Pavel Savchenko, Din Zelikovich, Hadassah Algavi Sinai, Roi Baer, and Daniel Mandler. The Effect of the Capping Agents of Nanoparticles on Their Redox Potential. *JACS*, in press, June 2024.

[4] Omer Haggag, Roi Baer, Sanford Ruhman, and Anna I. Krylov. Revisiting the benzene excimer using [2,2] paracyclophane model system: Experiment and theory. *J Chem Phys*, 160(12):124111, March 2024.

[5] Sayak Adhikari and Roi Baer. Weak second-order quantum state diffusion unraveling of the Lindblad master equation. *The Journal of Chemical Physics*, 160(6):064107, February 2024.

[6] Leopoldo Mejía, Jia Yin, David R. Reichman, Roi Baer, Chao Yang, and Eran Rabani. Stochastic Real-Time Second-Order Green's Function Theory for Neutral Excitations in Molecules and Nanostructures. *J. Chem. Theory Comput.*, 19(16):5563–5571, August 2023.

[7] Ming Chen, Roi Baer, and Eran Rabani. Structure optimization with stochastic density functional theory. *The Journal of Chemical Physics*, 158(2):024111, January 2023.

[8] Vladimir U. Nazarov and Roi Baer. High-frequency limit of spectroscopy. *The Journal of Chemical Physics*, 157(8):084112, August 2022.

[9] Ben Shpiro, Marcel David Fabian, Eran Rabani, and Roi Baer. Forces from Stochastic Density Functional Theory under Nonorthogonal Atom-Centered Basis Sets. *Journal of Chemical Theory and Computation*, 18(3):1458–1466, March 2022.

[10] Marcel D. Fabian, Ben Shpiro, and Roi Baer. Linear Weak Scalability of Density Functional Theory Calculations without Imposing Electron Localization. *Journal of Chemical Theory and Computation*, page acs.jctc.1c00829, March 2022.

[11] Wenjie Dou, Joonho Lee, Jian Zhu, Leopoldo Mejía, Roi Baer, and Eran Rabani. Time-Dependent Second-Order Green's Function Theory for Neutral 2 Excitations. *Journal of Chemical Theory and Computation*, page 12, 2022.

[12] Dror M. Bittner, Krishnendu Gope, Ester Livshits, Roi Baer, and Daniel Strasser. Sequential and concerted C–C and C–O bond dissociation in the Coulomb explosion of 2-propanol. *The Journal of Chemical Physics*, 157(7):074309, August 2022.

[13] Roi Baer, Daniel Neuhauser, and Eran Rabani. Stochastic Vector Techniques in Ground-State Electronic Structure. *Annual Review of Physical Chemistry*, 73(1):12.1–12.18, April 2022.

[14] Krishnendu Gope, Ester Livshits, Dror M. Bittner, Roi Baer, and Daniel Strasser. An "inverse" harpoon mechanism. *Science Advances*, 8(39):eabq8084, September 2022. Publisher: American Association for the Advancement of Science.

[15] 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.

[16] 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 ntls.10022, July 2021.

[17] 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.

[18] 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.

[19] Eitam Arnon, Eran Rabani, Daniel Neuhauser, and Roi Baer. Efficient Langevin dynamics for "noisy" forces. *J. Chem. Phys.*, 152(16):161103, April 2020.

[20] 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.

[21] 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.

[22] 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.

[23] 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.

[24] 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.

[25] Ming Chen, Roi Baer, Daniel Neuhauser, and Eran Rabani. Energy window stochastic density functional theory. *J. Chem. Phys.*, 151(11):114116, September 2019.

[26] 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.

[27] 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.

[28] 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.

[29] 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.

[30] 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.

[31] 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.

[32] 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.

[33] 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.

[34] 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.

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[40] Vojtěch Vlček, Roi Baer, Eran Rabani, and Daniel Neuhauser. Simple eigenvalue-self-consistent δGW0. *J. Chem. Phys.*, 149(17):174107, November 2018.

[41] 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.

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[44] 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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[47] 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.

[48] 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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[52] 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.

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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. Subotnik, Troy Van Voorhis, John M. Herbert, Anna I. Krylov, Peter M. W. Gill, and Martin Head-Gordon. Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Mol. Phys.*, 113(2):184–215, 2015.

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[59] 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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[61] David A Egger, Shira Weissman, Sivan Refaely-Abramson, Sahar Sharifzadeh, Matthias Dauth, Roi Baer, Stephan Ku mmel, 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.

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