July 24, 2020

Curriculum Vitae - Barak Hirshberg

Senior Lecturer (starting 2021), Tel Aviv University

Personal details

Israeli citizen, born September 5th, 1988 in Jerusalem, Israel.
E-Mail: barakh@ethz.ch; Scopus ID: 55008249000; Researcher ID: J-4518-2016.
Google Scholar: https://scholar.google.co.il/citations?user=4x2O7dcAAAAJ&hl=en
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Education

2014-2018: Ph.D. in Chemistry, Hebrew University of Jerusalem. Thesis supervisor: Prof. R.B. Gerber. Dissertation Title: Interactions, Spectroscopy and Dynamics of Many-Atom Systems.

2012-2014: M.Sc. (within the direct PhD track) in Physical and Theoretical Chemistry, Hebrew University of Jerusalem. Thesis supervisor: Prof. R.B. Gerber.

2006-2009: B.Sc. (*magna cum laude*) in Chemistry in the Amirim – Natural Sciences honors program, the Hebrew University of Jerusalem.

Academic Appointments

2021-today: Senior Lecturer, School of Chemistry, Tel Aviv University.

2018-2020: Rothschild Postdoctoral Fellow, ETH Zurich. Host: Prof. M. Parrinello.

Teaching

2015-2018: Teaching Assistant, Introduction to the Chemical Bond (69311), Physical Chemistry C (69601).

Military Service

2009-2015: IDF (Captain), Research and Development in RAFAEL Theoretical Physics group.

Honors and Awards

1. **2018-2019:** Rothschild Fellow, Yad-Hanadiv foundation.
2. **2017:** Israel Chemical Society Prize for an Excellent Graduate Student.
3. **2016:** Excellent teaching assistant (based on students' evaluations), Faculty of Science, Hebrew University of Jerusalem.
4. **2016:** USA-Israel Binational Science Foundation (BSF) Prof. Rahamimoff Travel Grants for Young Scientists.
5. **2015-2018:** Adams Fellow of the Israel Academy of Sciences and Humanities.
6. **2014:** The Lise Meitner-Minerva Center Junior Award for an outstanding work in computational quantum Chemistry.
7. **2012:** Giora Y. Yashinski memorial award for excellent M.Sc. and Ph.D. students.
8. **2009:** Graduated with B.Sc. in Chemistry *magna cum laude*.
9. **2008-2009:** Amirim – Natural Sciences Honors Scholarship.
10. **2007-2008:** Dean's list for excellent B.Sc. student.
11. **2008:** Prof. P. Elving memorial award for excellence in Analytical Chemistry.
12. **2007:** The Dean's Award for excellent B.Sc. students.

Peer-Reviewed Publications

1. D. Mandelli, **B. Hirshberg** and M. Parrinello, *Metadynamics of Paths*, Phys. Rev. Lett. 125 (2020) 026001.
2. **B. Hirshberg**, M. Invernizzi and M. Parrinello, *Path Integral Molecular Dynamics for Fermions: Alleviating the Sign Problem with the Bogoliubov Inequality*, Communication in J. Chem. Phys. 152 (2020) 171102.
3. **B. Hirshberg**, V. Rizzi and M. Parrinello, *Path Integral Molecular Dynamics for Bosons*, Proc. Natl. Acad. Sci. U.S.A. 116 (2019) 21445-21449.
4. L. Sagiv, **B. Hirshberg** and R.B. Gerber, *Hydrogenic Stretch Spectroscopy of Glycine-Water Complexes: Anharmonic Ab Initio Classical Separable Potential Calculations*, J. Phys. Chem. A 123 (2019) 8377-8384.
5. **B. Hirshberg**, E. Rossich Molina, A.W. Götz, A.D. Hammerich, G.M. Nathanson, T.H. Bertram, M.A. Johnson and R.B. Gerber, *N_2O_5 at water surfaces: binding forces, charge separation, energy accommodation and atmospheric implications*, Phys. Chem. Chem. Phys. 20 (2018) 17961-17976.
6. **B. Hirshberg**, R.B. Gerber and A.I. Krylov, *Autocorrelation of electronic wave-functions: a new approach for describing the evolution of electronic structure in the course of dynamics*, Mol. Phys. 116 (2018) 2512-2523.
7. L. Sagiv, **B. Hirshberg**, R.B. Gerber, *Anharmonic Vibrational Spectroscopy Calculations Using the Ab Initio CSP Method: Applications to H_2CO_3, $(H_2CO_3)_2$, H_2CO_3-H_2O and Isotopologues*, Chem. Phys. 514 (2018) 44-54.
8. P.J. Kelleher, F.S. Menges, J.W. DePalma, J.K. Denton, M.A. Johnson, G.H. Weddle, **B. Hirshberg** and R.B. Gerber *Trapping and Structural Characterization of the $XNO_2{\cdot}NO3^-$ (X = Cl, Br, I) Exit Channel Complexes in the Water-Mediated X^- + N_2O_5 Reactions with Cryogenic Vibrational Spectroscopy,* J. Phys. Chem. Lett. 8 (2017) 4710-4715.
9. **B. Hirshberg** and R.B. Gerber, *Mean-Field Methods for Time-Dependent Quantum Dynamics of Many-Atom Systems*, Advances in Quantum Chemistry, 75 (2017) 1-26**.**
10. **B. Hirshberg**, L. Sagiv, and R. B. Gerber**,** *Approximate Quantum Dynamics using Ab Initio Classical Separable Potentials: Spectroscopic Applications***,** J. Chem. Theory Comput. 13 (2017) 982–991.
11. **B. Hirshberg** and R.B. Gerber *Formation of Carbonic Acid in Impact of CO_2 on Ice and Water*, J. Phys. Chem. Lett. 7 (2016) 2905-2909.
12. R.B. Gerber, D. Shemesh, M.E. Varner, J. Kalinowski and **B. Hirshberg,** *Ab Initio and Semi-empirical Molecular Dynamics in Isolated Molecules and in Clusters*, Perspective in Phys. Chem. Chem. Phys. 16 (2014) 9760-9775.
13. D. Furman, R. Kosloff, F. Dubnikova, S.V. Zybin, W.A. Goddard III, N. Rom, **B. Hirshberg** and Y. Zeiri, *Decomposition of Condensed Phase Energetic Materials: Interplay between Uni- and Bimolecular Mechanisms*, J. Am. Chem. Soc. 136 (2014) 4192-4200.
14. **B. Hirshberg**, R.B. Gerber and A.I. Krylov**,** *Calculations predict a stable molecular crystal of N_8*, Nature Chem. 6 (2014) 52-56.
    Highlighted in Chemistry World: *https://www.chemistryworld.com/news/calculations-predict-stable-eight-nitrogen-molecule/6901.article*
15. N. Rom**, B. Hirshberg**, Y. Zeiri, D. Furman, S.V. Zybin, W.A. Goddard III and R. Kosloff, *First Principles Based Reaction Kinetics for Decomposition of Hot Dense Liquid TNT from ReaxFF Multiscale Reactive Dynamics Simulations*, J. Phys. Chem. C 117 (2013) 21043–21054.
16. **B. Hirshberg** and C. Denekamp, *First Principles Prediction of an Insensitive High Energy Density Material*, Phys. Chem. Chem. Phys. 15 (2013) 17681-17688.

17. **B. Hirshberg** and R.B. Gerber, *Decomposition mechanisms and dynamics of N_6: partial charges and bond orders along classical trajectories,* Chem. Phys. Lett. 531 (2012) 46-51.

Conference Presentations and Seminars

Invited

1. *Path integral molecular dynamics for bosons and fermions: From ultracold atoms to quantum dots, Virtual Conference on Theoretical Chemistry (VCTC2020), July 2020. Organized by Prof. T.J. Martinez, Stanford University. Online due to COVID-19 pandemic.*
2. *Path integral molecular dynamics for bosons and fermions: From ultracold atoms to quantum dots*, Chemistry department seminar, Bar-Ilan University, January 2020, Israel.
3. *Path integral molecular dynamics for bosons and fermions: From ultracold atoms to quantum dots*, Theoretical Chemistry seminar, ETH Zurich, January 2020, Switzerland
4. *Path Integral Molecular Dynamics for Bosons*, BEC center seminar, Physics department, University of Trento, December 2019, Trento, Italy.
5. *Path Integral Molecular Dynamics for Indistinguishable Particles*, Theoretical Chemistry seminar, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, November 2019, Prague, Czech Republic.
6. *Path Integral Molecular Dynamics for Bosons*, 10th congress of the international society of theoretical chemical physics (ISTCP-X), July 2019, Tromso, Norway.
7. *Interactions, Spectroscopy and Dynamics of Many-Atom Systems*, Physical and Analytical Chemistry Seminar, Technion, June 2018, Haifa, Israel.
8. *Formation of carbonic acid from the impact of CO_2 on water*, AirUCI seminar, the University of California Irvine, June 2015, Irvine, CA, USA.

Contributed

1. *Path integral molecular dynamics for bosons and fermions: From ultracold atoms to quantum dots*, 85th annual meeting of the Israel Chemical Society, February 2020, Jerusalem, Israel.
2. *Path integral molecular dynamics for bosons and fermions: From ultracold atoms to quantum dots*, 65th annual meeting of the Israel Physical Society (IPS2020), February 2020, Rehovot, Israel.
3. *Path Integral Molecular Dynamics for Cold Bosons*, Molecular and Materials Simulations at the Turn of the Decade: Celebrating 50 Years of CECAM, September 2019, Lausanne, Switzerland.
4. *Towards Path Integral Molecular Dynamics Simulations of Bosons and Fermions*, Workshop on Theoretical Chemistry, February 2019, Mariapfarr, Austria.
5. *Quantum Vibrational Spectroscopy of Biomolecules using ab initio Classical Separable Potentials*, 9th Graduate students conference of the Israel chemical society, October 2017, the Hebrew University of Jerusalem. ***Winner of best oral presentation award.***
6. *Quantum Vibrational Spectroscopy of Amino Acids using Classical Separable Potentials*, Gordon Research Seminar on Molecular Interactions and Dynamics, July 2016, Stonehill College, Easton, MA, USA.
7. *PHYS: Theoretical Prediction of Crystalline N_8*, 247th ACS National Meeting & Exposition, March 2014, Dallas, TX, USA.
8. *COMP: First Principles Prediction of an Insensitive High Energy Density Material*, 247th ACS National Meeting & Exposition, March 2014, Dallas, TX, USA.

Other Noteworthy Activities and Skills

1. Elected chair for Gordon Research Seminar on Molecular Interaction and Dynamics, July 2018, Stonehill College, Easton, MA, USA.
2. Reviewer for: Journal of Physical Chemistry Letters, Physical Chemistry Chemical Physics, New Journal of Chemistry, International Journal of Quantum Chemistry, Molecular Physics and Communications Chemistry.