

Curriculum Vitae

Barak Hirshberg

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Personal information

Date of Birth: September 5th, 1988. City of Birth: Jerusalem. Nationality: Israeli.

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Ma'ale Adumim, Israel

Education

2014 - **Ph.D. Student**, Theoretical and Physical Chemistry, Department of Physical Chemistry and the Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Jerusalem 91904, Israel.

- *Ph.D. Thesis Supervisor: Prof. R. Benny Gerber*

2012 - 2014 **Master of Science (Direct Ph.D. track)**, Theoretical and Physical Chemistry, Department of Physical Chemistry and the Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Jerusalem 91904, Israel. **Courses GPA: 95.20. M.Sc. exam grade: 99.**

- *M.Sc. Advisor: Prof. R. Benny Gerber*

2007- 2009 - **Bachelor of Science (*magna cum laude*)**, Chemistry, Hebrew University of Jerusalem, Jerusalem 91904, Israel. **GPA: 95.74.**

- *Member of the "Amirim" Natural Sciences Honors Program*
- *Thesis Title: Decomposition Pathways and Dynamics of N_4*
- *Thesis Supervisor: Prof. R. Benny Gerber*
- *Thesis grade: 98.0*

Awards and Distinctions

- *2015-2018 Adams Fellow of the Israel Academy of Sciences and Humanities*

- 2014- *The Lise Meitner-Minerva Center Junior Award for an outstanding work in computational quantum Chemistry*
- 2012- *Giora Y. Yashinski memorial award for excellent M.Sc. and Ph.D. students*
- 2009- *Graduated with B.Sc. in Chemistry magna cum laude*
- 2007-2008 "*Amirim*" *Natural Sciences Honors Scholarship*
- 2007-2008 *Dean's list for excellent B.Sc. student*
- 2008- *Prof. P. Elving memorial award for excellence in Analytical Chemistry*
- 2007- *The Dean's Award for excellent B.Sc. students*

Peer Reviewed Publications

1. **B. Hirshberg** and R.B. Gerber, *Decomposition mechanisms and dynamics of N₈: partial charges and bond orders along classical trajectories*, **Chem. Phys. Lett.** **531** (2012) 46-51.
2. **B. Hirshberg** and C. Denekamp, *First Principles Prediction of an Insensitive High Energy Density Material*, **Phys. Chem. Chem. Phys.** **15** (2013) 17681-17688.
3. 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.
4. **B. Hirshberg**, R.B. Gerber and A.I. Krylov, *Calculations predict a stable molecular crystal of N₈*, **Nature Chem.** **6** (2014) 52-56.
 - a. **Highlight in Chemistry World (RSC journal)**
<http://www.rsc.org/chemistryworld/2013/12/calculations-predict-stable-eight-nitrogen-molecule>
5. 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.
6. 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.
7. **B. Hirshberg** and R.B. Gerber *Formation of Carbonic Acid in Impact of CO₂ on Ice and Water*, **J. Phys. Chem. Lett.** **7** (2016) 2905-2909.

Poster Presentations

- 1. B. Hirshberg** and R.B. Gerber, Decomposition pathways and dynamics of new polynitrogen molecules, Fritz Haber center biannual symposium, 2009, Kibbutz Ma'ale HaHamisha, Israel.
- 2. B. Hirshberg** and R.B. Gerber, *Decomposition pathways and dynamics of new polynitrogen molecules*, Gordon Research Conference on Physics and Chemistry of matrix isolated species, July 2009, Oxford, UK.
- 3. B. Hirshberg** and R.B. Gerber, *Decomposition mechanisms and dynamics of N_6 : partial charges and bond orders along classical trajectories*, Quantum Dynamics, A conference in Honor of W.H. Miller's 70th birthday, 9-12 January 2012, Berkeley, CA, USA.
- 4. B. Hirshberg** and R.B. Gerber, *Decomposition mechanisms and dynamics of N_6 : partial charges and bond orders along classical trajectories*, Theory and Applications of Computational Chemistry 2012 (TACC2012), 2-7 September 2012, Pavia, Italy.
- 5. B. Hirshberg**, A.I. Krylov and R.B. Gerber, *Prediction of Crystalline N_8* , Molecular Quantum Mechanics 2013 (MQM2013), A conference in Honor of R.J. Bartlett, 2-7 June 2013, Lugano, Switzerland.
- 6. B. Hirshberg** and R.B. Gerber, *Formation of Carbonic Acid in the Impact of CO_2 on Water*, Computational Molecular Sciences 2015 (CMS2015), 15-18 March 2015, Warwick, UK.
- 7. B. Hirshberg** and R.B. Gerber, *Formation of Carbonic Acid in the Impact of CO_2 on Water*, The Batsheva de Rothschild Seminar on: Current Challenges in Chemical Dynamics: From Exotic Novel Species to Macromolecules, 12-15 October, 2015, Neve Ilan, Israel. **Winner of 2nd best poster award.**
- 8. B. Hirshberg** and R.B. Gerber, *Formation of Carbonic Acid in the Impact of CO_2 on Ice and Water*, Gordon Research Conference on Molecular Interactions and Dynamics, July 2016, Stonehill College, Easton, MA, USA.

Conference Talks

- 1. B. Hirshberg**, A.I. Krylov and R.B. Gerber, PHYS: Theoretical Prediction of Crystalline N_8 , 247th ACS National Meeting & Exposition, March 2014, Dallas, TX, USA.
- 2. B. Hirshberg** and C. Denekamp, COMP: First Principles Prediction of an Insensitive High Energy Density Material, 247th ACS National Meeting & Exposition, March 2014, Dallas, TX, USA.

3. B. Hirshberg, L. Sagiv and R.B. Gerber, 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.

Military Service

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

References

References will be given upon request.