CURRICULUM VITAE
Dr. Michal Ben-Nun

EDUCATION

Hebrew University of Jerusalem, Israel: Ph.D., 1996, Theoretical Chemistry
Hebrew University of Jerusalem, Israel: B.Sc., 1990, Chemistry

EXPERIENCE

Research Scientist November 2011-todate
Predictive Science, San Diego, CA.

- Develop predictive capabilities for Influenza Dynamics forecasting.

Research Scientist Oct. 2007-October 2011
Spectral Associates, San Diego, CA.

- Key developer for a Department of Defense sponsored computational chemistry research project, including debugging, benchmarking, and deployment at the HPC systems at SDSC.

Off-Site Consultant, October 2003 – October 2007
University of Illinois, Urbana IL.

- As a member of an NSF funded Cyber Infrastructure Project investigated the integration and use of BABEL (a scientific interface description language) for physical science applications. Integrated proprietary molecular dynamics code with GAMESS.

Lecturer, September 2002 – September 2003
Santa Clara University, Santa Clara CA.

- Taught a three-part General Chemistry lecture and lab sequence to science and engineering majors.

Visiting Assistant Professor, September 1999 – August 2002
University of Illinois, Urbana IL.

- Developed and interfaced a proprietary molecular dynamics code with commercial *ab initio* and semi-empirical electronic structure programs. Code was deployed at the HPC systems at NCSA.

Postdoctoral Fellow, May 1997 – September 1999
University of Illinois, Urbana IL.

- Developed and interfaced an *ab initio* electronic structure code to NAMD: a parallel object oriented molecular dynamics code. Code was used to study retinal analogs using the HPC systems at NCSA and the NIH Resource for Macromolecular Modeling and Bioinformatics.

Fulbright and Rothchild Postdoctoral Fellow, September 1995 – May 1997
University of California San Diego, San Diego, CA.

- As a member of an experimental high-energy physics and chemistry group developed and implemented theoretical and computational tools for modeling ultra-fast x-ray and electron diffraction patterns.

Graduate Student, September 1990 – September 1995
The Hebrew University of Jerusalem, Jerusalem, Israel.

- Under the guidance of Prof. R. D. Levine, developed and applied analytical and computational tools to the study of bio-molecular chemical reactions in solutions.

PUBLICATIONS

1. K. G. Rollin, M. W. J. Bromley, M. Ben-Nun, G. A. Gallup, and P. W. Langhoff, Convergence of Even Tempered Slater-Based Configuration-Interaction Calculations (in preparation) 2011.
2. K. G. Rollin, M. W. J. Bromley, M. Ben-Nun, G. A. Gallup, and P. W. Langhoff, Open-Shell Fock Orbitals in Configuration-Interaction calculations of Atomic Spectra (in preparation) 2011.
3. M. Ben-Nun, J. D. Mills, R. J. Hinde, C. L. Winstead, J. A. Boatz, G. A. Gallup, and P. W. Langhoff, Atomic-Spectral Representations of Molecular Electronic Structure: Metric Matrices and Atomic-Product Composition of Molecular Eigenfunctions, *J. Phys. Chem.* A **113**, 7687 (2009).
4. M. Ben-Nun and T. J. Martinez, A Continuous Spawning Method for Nonadiabatic Dynamics: Validation for the Zero-Temperature Spin-Boson Problem, *Isr. J. Chem.* **47**, 75 (2007).
5. A. Toniolo, B. Levine, A. Thompson, J. Quenneville, M. Ben-Nun, J. Owens, S. Olsen, L. Manohar, and T. J. Martinez, Photochemistry from First Principles and Direct Dynamics, *Computational Methods in Organic Photochemistry*, Ed. A. Kutateladze (New York, Marcel-Dekker, 2005).
6. A. Toniolo, M. Ben-Nun and T. J. Martinez, Optimization of Conical Intersections with Floating Occupation Semiempirical Configuration Interaction Wavefunctions, *J. Phys. Chem.* A **106**, 4679 (2002).
7. M. Ben-Nun and T. J. Martinez, *Ab Initio* Quantum Molecular Dynamics, *Adv. Chem. Phys.* **121**, 439 (2002).
8. M. Ben-Nun, F. Molnar, K. Schulten and T. J. Martinez, Intersection Topography and Bond Selectivity in Photoisomerization Reactions, *Proc. Natl. Acad. Sci. USA* **99**, 1769 (2002).
9. M. D. Hack, A. M. Wensmann, D. G. Truhlar, M. Ben-Nun and T. J. Martinez, Comparison of Full Multiple Spawning, Trajectory Surface Hopping, and Converged Quantum Mechanics for Electronically Nonadiabatic Dynamics, *J. Chem. Phys.* **115**, 1172 (2001).
10. J. Quenneville, M. Ben-Nun and T. J. Martinez, Photochemistry from First Principles: Advances and Future Prospects, *J. Photochem. Photobiol.* **144**, 229 (2001).
11. M. Ben-Nun and T. J. Martinez, Photodynamics of Ethylene: *Ab Initio* Studies of Conical Intersections, *Chem. Phys.* **259**, 237 (2000).

12. M. Ben-Nun and T. J. Martinez, Direct Observation of the Disrotatory Ring-Opening Reaction of Cyclobutene Using *Ab Initio* Molecular Dynamics, *J. Am. Chem. Soc.* **122**, 6299 (2000).
13. M. Ben-Nun, J. Quenneville and T. J. Martinez, *Ab Initio* Multiple Spawning: Photochemistry from First Principles Quantum Molecular Dynamics, *J. Phys. Chem.* A (Feature Article) **104**, 5161 (2000).
14. F. Molnar, M. Ben-Nun, T. J. Martinez and K. Schulten, Characterization of a Conical Intersection between the Ground and First Excited State for a Retinal Analog, *J. Mol. Struct.* (THEOCHEM) **506**, 169 (2000).
15. M. Ben-Nun and T. J. Martinez, A Multiple Spawning Approach to Tunneling Dynamics, *J. Chem. Phys.* **112**, 6113 (2000).
16. M. Ben-Nun and T. J. Martinez, Electronic Absorption and Resonance Raman Spectroscopy from *Ab Initio* Quantum Molecular Dynamics*, J. Phys. Chem.* A **103**, 10517 (1999).
17. M. Ben-Nun and T. J. Martinez, Semiclassical Tunneling Rates from *Ab Initio* Molecular Dynamics, *J. Phys. Chem.* A **103**, 6055 (1999).
18. M. Ben-Nun and T. J. Martinez, Exploiting Temporal non-locality to Remove Scaling Bottlenecks in Non-adiabatic Quantum Dynamics, *J. Chem. Phys.* **110**, 4134 (1999).
19. M. Ben-Nun and T. J. Martinez, *Ab Initio* Multiple Spawning of Photoinduced *cis-trans* Isomerization in Ethylene, *Chem. Phys. Lett.* **298**, 57 (1998).
20. M. Ben-Nun and T. J. Martinez, Electronic Energy Funnels in *cis-trans* Photoisomerization of Retinal Protonated Schiff Base, *J. Phys. Chem.* A **102**, 9607 (1998).
21. M. Ben-Nun, F. Molnar, H. Lu, J. C. Phillips, T. J. Martinez and K. Schulten, Quantum Dynamics of Retinal's Femtosecond Photoisomerization in Bacteriorhodopsin, *Faraday Discussions* **110**, 447 (1998).
22. M. Ben-Nun and T. J. Martinez, Direct Evaluation of the Pauli Repulsion Energy using "Classical" Wavefunctions in Hybrid Quantum/Classical Potential Energy Surfaces, *Chem. Phys. Lett.* **290**, 289 (1998).
23. M. Ben-Nun and T. J. Martinez, Validation of the Multiple Spawning Method for Nonadiabatic Dynamics in a Multidimensional Model Problem, *J. Chem. Phys.* **108**, 7244 (1998).
24. M. Ben-Nun, J. Cao and K. R. Wilson, Ultrafast X-Ray and Electron Diffraction: Theoretical Considerations, *J. Phys. Chem.* A **101**, 8743 (1997).
25. M. Ben-Nun, T. J. Martinez and R. D. Levine, Dynamical Stereochemistry on Several Electronic States: A Computational Study of $Na^* + H_2$, *J. Phys. Chem.* A **101**, 7522 (1997).
26. T. J. Martinez, M. Ben-nun and R. D. Levine, Molecular Collision Dynamics on Several Electronic States, *J. Phys. Chem.* A **101**, 6389 (1997).
27. M. Ben-Nun, T. J. Martinez and R. D. Levine, Multiple Traversals of a Conical Intersection: Electronic Quenching in $Na^* + H_2$, *Chem. Phys. Lett.* **270**, 319 (1997).

28. J. K. Krause, K. J. Schafer, M. Ben-Nun, and K. R. Wilson, Creating and Detecting Shaped Rydberg Wavepackets, *Phys. Rev. Lett.* **79**, 4978 (1997).

29. M. Ben-Nun, T. J. Martinez, P. M. Weber and K. R. Wilson, Direct Imaging of Excited Electronic States Using Diffraction Techniques: Theoretical Considerations, *Chem. Phys. Lett.* **262**, 405 (1996).

30. M. Ben-Nun and R. D. Levine, On the Zero Point Energy in Classical Trajectory Computations, *J. Chem. Phys.* **105**, 8136 (1996).

31. C. P. J. Barty, M. Ben-Nun, T. Guo, F. Raksi, C. Rose-Petruck, J. Squier, K. R. Wilson, V. V. Yakovlev, P. M. Weber, Z. Jiang, A. Ikhelf and J. –C. Kieffer, Ultrafast X-ray Diffraction and Absorption, in *Time Resolved Electron and X-Ray Diffraction*, Eds. P. M. Rentzepis and J. Helliwell (Oxford University Press, New York) p. 44-70 (1998).

32. M. Ben-Nun, R. D. Levine and G. R. Fleming, Solvent Induced Nonadiabatic Transitions in Iodine: An Ultrafast Pump-Probe Computational Study, *J. Chem. Phys.* **105**, 3035 (1996).

33. T. J. Martinez, M. Ben-Nun and R. D. Levine, Multi Electronic State Molecular Dynamics: A Wave Function Approach with Application, *J. Phys. Chem.* **100**, 7884 (1996).

34. T. J. Martinez, M. Ben-Nun and G. Ashkenazi, Classical/Quantal Method for Multistate Dynamics: A Computational Study, *J. Chem. Phys.* **104**, 2847 (1996).

35. M. Ben-Nun, R. D. Levine, D. M. Jonas and G. R. Fleming, Prompt Solvent Induced Electronic Predissociation of Femtosecond Pumped Iodine: A Computational Study, *Chem. Phys. Lett.* **245**, 629 (1995).

36. M. Ben-Nun and R. D. Levine, Short-Time Dynamics on Several Electronic States: Formalism and Computational Study of I_2 in Rare Gas Solvents, *Chem. Phys.* **201**, 163 (1995).

37. X. Wang, M. Ben-Nun and R. D. Levine, Peripheral Dynamics of the Cl + CH_4 ® HCl + CH_3 Reaction. A Classical Dynamics Computation, *Chem. Phys.* **197**, 1 (1995).

38. M. Ben-Nun and R. D. Levine, Kinetics and Dynamics of Reactions in Liquids, *Int. Rev. Phys. Chem.* **14**, 215 (1995).

39. T. Raz, I. Scheck, M. Ben-Nun, U. Even, J. Jortner and R. D. Levine, Dissociation Dynamics of Diatomic Molecules Embedded in Impact Heated Rare Gas Clusters, *J. Chem. Phys.* **101**, 8606 (1994).

40. M. Ben-Nun and R. D. Levine, Conservation of Zero Point Energy in Classical Trajectory Computations by a Simple Semiclassical Correspondence, *J. Chem. Phys.* **101**, 8768 (1994).

41. M. Ben-Nun, T. Raz and R. D. Levine, Ballistic and Dissociative Collisions of a Rare Gas Atom with a Halogen Molecule, *Chem. Phys. Lett.* **220**, 291 (1994).

42. M. Ben-Nun, and R. D. Levine, Liquid State Control of Chemical Reactions: Toward a Molecular Description, *Acc. Chem. Res.* **27**, 166 (1994).

43. M. Ben-Nun, and R. D. Levine, Ion-Molecule Recombination and Other Activationless Processes in Solution: Foundations of a Capture Model, *J. Chem. Phys.* **100**, 3594 (1994).

44. M. Ben-Nun, and R. D. Levine, Stabilization of Ion-Molecule Pairs by Solvation, *Chem. Phys. Lett.* **214**, 175 (1993).

45. U. Even, M. Ben-Nun and R. D. Levine, Time Evolution of Very High Rydberg States of Large Aromatic Molecules: A Kinematic Analysis, *Chem. Phys. Lett.* **210**, 416 (1993).

46. M. Ben-Nun, M. Brouard, J. P. Simons and R. D. Levine, Peripheral Chemical Reactions, *Chem. Phys. Lett.* **210**, 423 (1993).

47. M. Ben-Nun, and R. D. Levine, Coherent Vibrational Spectroscopy of Barrier Descent Dynamics, *Chem. Phys. Lett.* **203**, 450 (1993).

48. M. Ben-Nun, and R. D. Levine, Direct Exchange Reactions in a Liquid: The Cage Effect and Its Spectroscopic Manifestations, *J. Phys. Chem.* **97**, 2334 (1993).

49. M. Ben-Nun, and R. D. Levine, Dynamics of Bimolecular Reactions in Solution: A Nonadiabatic Activation Model, *J. Chem. Phys.* **97**, 8341 (1992).

50. M. Ben-Nun, and R. D. Levine, An Approximate Solution of the Fokker-Planck Equation for Reactions in Condensed Phases, *Chem. Phys. Lett.* **192**, 472 (1992).

51. M. Ben-Nun, and R. D. Levine, The Cage effect and Energetic and Steric Requirements of Elementary Bimolecular Reactions in Condensed Phases, *J. Phys. Chem.* **96**, 1523 (1992).

52. O. M. Becker, M. Ben-Nun and A. Ben-Shaul, Reactants Segregation in the Steady State A + B ® O Reaction on Surfaces, *J. Phys. Chem.* **95**, 4803 (1991).

53. O. M. Becker, M. Ben-Nun and A. Ben-Shaul, Spatial and Temporal Correlations in Surface Reactions, in *Correlation and Connectivity in Constrained Geometries*, Eds. H. E. Stanley and N. Ostrowsky (Kluwer Academic Press, Dordrecht), p 305-307 (1990).