

Naomi Rom - Curriculum Vitae

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Personal Information

Name: Naomi Rom

Born: Israel, 1966

Tel: 0524-291-829

Army Service: 1984-1986

Education

- **1989-1995: D.Sc. in Chemistry, Technion – Israel Institute of Technology, Haifa.**

Dissertation topic: "Determination of Tunneling Rates through Potential Barriers". Thesis supervisor: Prof. Nimrod Moiseyev.

Developed several algorithms to calculate chemical reaction rates in systems supporting resonances. Used complex scaling methods with grid algorithms and matrix calculations.

- **1986–1989: B. Sc. in Chemistry (Cum Laude), Technion – Israel Institute of Technology, Haifa.**
- **1983-1984: Foothill Junior College, Los Altos Hills, California.**
- **1982-1983: Paly High School, Palo Alto, California.**
- **1978-1982: Alliance High School, Haifa.**

Teaching Experience

- **1989-1995: Teaching assistant in undergraduate and graduate Chemistry faculty courses in the Technion.**

The courses include: general chemistry, physical chemistry, quantum chemistry, and computational chemistry, and physical chemistry lab instructor.

Employment Experience

- **12/2003–present: Rafael.**
Tasks leader in various projects.
- **10/2009-12/2010: Fritz Haber Institute for Molecular Dynamics, Hebrew University, Jerusalem.**

Visiting Scholar, collaboration with Prof. Ronnie Kosloff.

Reactive molecular dynamics simulations

- **12/2000-9/2003: OpTun Ltd, Haifa.**

Head of Architecture and Data Management group.

Work topics include: Optical devices design; Architecture design of various integrated optical devices; Switching algorithms and functionality; Products layout; Packaging adaptation.

- **9/1997-11/2000: Rafael.**

Material properties research.

- **6/1995-6/1997: University of California at Los Angeles (UCLA).**

Postdoctoral Fellow with Prof. Daniel Neuhauser.

Developed a new Complex Monte Carlo electronic structure algorithm and applied it to several molecular systems.

Awards and Scholarships

- **2011 and 2012:** Special award for excellent fulfillment of an assignment, Rafael.
- **2009:** Special award for excellent team achievement, Rafael.
- **2008:** Special award as a subject leader, Rafael.
- **2000-2003:** Katzir Fellowship.
- **1994:** Special excellence scholarship, the Gutwirth Foundation, Technion.
- **1991:** Regular excellence scholarship, the Gutwirth Foundation, Technion.
- **1991:** Travel and participation scholarship for first EPS Southern European School of Physics on “Dynamical Processes in Molecular Physics”.
- **1988: (1)** Kolthoff Prize, Technion; **(2)** Amos de Shalitt scholarship for summer school, Weizmann Institute of Science.
- **1987 and 1988:** The Technion President Prize for excellence in studies.
- **1986:** The Technion Dean Prize for excellence in studies.

List of Publications

1. "Decomposition of Condensed Phase Energetic Materials: Interplay between Uni- and Bimolecular Mechanisms", D. Furman, R. Kosloff, F. Dubnikova, S. V. Zybin, W. A. Goddard, III, N. Rom, B. Hirshberg, and Y. Zeiri, *J. Am. Chem. Soc.* 2014, 136, 4192-4200.
2. "First-Principles-Based Reaction Kinetics for Decomposition of Hot, Dense Liquid TNT from ReaxFF Multiscale Reactive Dynamics Simulations", N. Rom, B. Hirshberg, Y. Zeiri, D. Furman, S.V. Zybin, W.A. Goddard, III, and R. Kosloff, *J. Phys. Chem. C* 2013, 117, 21043–21054.
3. "Density-Dependent Liquid Nitromethane Decomposition: Molecular Dynamics Simulations Based on ReaxFF", N. Rom, S.V. Zybin, A.C.T. van Duin, W.A. Goddard, Y. Zeiri, G. Katz, and R. Kosloff, *J. Phys. Chem. A* 2011, 115, 10181–10202.
4. "Shifted-contour auxiliary-field Monte Carlo for molecular electronic structure", N. Rom, E. Fattal, A. K. Gupta, E. A. Carter and D. Neuhauser, *J. Chem. Phys.* 1998, 109, 8241.
5. "Shifted-contour auxiliary-field Monte Carlo: Circumventing the sign difficulty for electronic-structure calculations", N. Rom, D.M. Charutz, and D. Neuhauser, *Chem. Phys. Lett.* 1997, 270, 382-386.
6. "Scattering matrix elements by a time independent wave packet complex scaling formalism", N. Rom, J. W. Pang, and D. Neuhauser, *J. Chem. Phys.* 1996, 105, 10436.
7. "Transition-state resonances by complex scaling – H+H₂ and H+MuH", N. Rom and N. Moiseyev, *J. Phys. Chem.* 1994, 98, 3398-3406.
8. "Absorbing boundary conditions by the partial integration exterior scaling method", N. Rom and N. Moiseyev, *J. Chem. Phys.* 1993, 99, 7703.
9. "Cumulative reaction probability by the complex coordinate scattering theory", N. Rom, V. Ryaboy and N. Moiseyev, *J. Chem. Phys.* 1993, 98, 6327.

10. "Thermal rate constants of multi-mode systems for the price of one: aziridine", N. Rom, V. Ryaboy and N. Moiseyev, Chem. Phys. Lett. 1993, 204, 175.
11. "Thermal rate constants in collinear atom transfer reactions by optimizing the position of the reactants/products dividing surface", J. Chem. Phys. 1992, 96, 8307.
12. "Tunneling rates in a two-dimensional symmetric double-well potential surface by the exterior scaling procedure", N. Rom, N. Moiseyev and R. Lefebvre, J. Chem. Phys. 1991, 95, 3562.
13. "Optical potentials by the complex coordinate method", N. Rom, N. Lipkin and N. Moiseyev, Chem. Phys. 1991, 151, 199-204.
14. "Tunneling rates in bound systems using smooth exterior complex scaling within the framework of the finite basis set approximation", N. Rom, E. Engdahl, and N. Moiseyev, J. Chem. Phys. 1990, 93, 3413.