

Shikha Nangia

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EDUCATION

- 2006 Ph. D. *University of Minnesota*
- 2000 M.S. in Chemistry, *Indian Institute of Technology (IIT)*
- 1998 B.S. in Chemistry, *University of Delhi*

PROFESSIONAL EXPERIENCE

2006–present **Postdoctoral Research** (Advisor: Prof. Barbara J. Garrison)

- Development of reactive Monte Carlo algorithm to study equilibrium properties of dissolution of minerals
- Ab-initio density functional calculations of dissolution rates for silicates and aluminosilicates as a function of pH
- Cyberinfrastructure– involved in constructing an integrated database and digital library for chemical kinetics data

TEACHING EXPERIENCE

- Co-instructor (Pennsylvania State University, 2008)
Taught lectures, homework assignments, lead classroom activities
 - CHEM 402: Course focusing on the chemistry in the environment of the atmosphere, natural waters, and the land surface
- Invited Lecture (Pennsylvania State University, 2007)
 - CHEM 529: Cyberinfrastructure
- Co-instructor (University of Minnesota, 2003)
 - Center for Teaching and Learning: Provided instructions in the International Faculty and TA Program, teaching English language and classroom communication strategies to Non-native English-speaking TAs
- Teaching Assistant (University of Minnesota, 2001–2003)
Conducted lab and pre-lab, experiment demonstrations, tutoring, and grading
 - CHEM 1011, 1021, and 1022: Introductory Chemistry, Chemical Principles I and II

HONORS

- Travel award, 236th ACS National Meeting, Philadelphia PA (2009)
- Awarded Scholarship to attend the ACS PRF summer school on *Computation, Simulation, and Theory in Chemistry, Chemical Biology, and Materials Chemistry*, June 11-18, 2005, Park City, Utah
- Nominated for the Overend award for graduate research in physical chemistry
- Ranked 3rd in the nation-wide entrance exam for admittance to the MS program in the Indian Institute of Technology, India
- Ranked 5th in Delhi University with more 200 colleges offering BS in Chemistry, India

- Ranked 1st in the High school examination leading over 250 students conducted by the Central Board of Secondary Examination, India

PUBLICATIONS

12. Advanced Monte Carlo approach to study evolution of quartz surface during the dissolution process, S. Nangia and B. J. Garrison, *J. Am. Chem. Soc.* **131**, 9538-9546 (2009).
11. Ab-initio study of dissolution of quartz from edge, kink, and surface sites, S. Nangia and B. J. Garrison, *Mol. Phys. (invited)*, **107**, 831-843 (2009).
10. Dissolution mechanisms of aluminosilicates, C. P. Morrow, S. Nangia and B. J. Garrison, *J. Phys. Chem. A*, **113**, 1343-1352 (2009).
9. Reaction rates and dissolution mechanisms of quartz as a function of pH, S. Nangia and B. J. Garrison, *J. Phys. Chem. A* **112**, 2077-2033 (2008).
8. Study of a family of 40 hydroxylated beta-cristobalite surfaces using empirical potential energy functions, S. Nangia, N. M. Washton, K. T. Mueller, J. D. Kubicki, and B. J. Garrison, *J. Phys. Chem. C* **111**, 5169-5177 (2007).
7. Direct calculation of coupled diabatic potential-energy surfaces for ammonia and mapping of a four-dimensional conical intersection seam, S. Nangia and D. G. Truhlar, *J. Chem. Phys.* **124**, 124309-13 (2006).
6. Non-Born-Oppenheimer molecular dynamics, A. W. Jasper, S. Nangia, CY. Zhu, and D. G. Truhlar, *Acc. Chem. Res.* **39** 101-108 (2006).
5. A new form of MgTa₂O₆ obtained by the molten salt method, A. K. Ganguly, S. Nangia, M. Thirumal, and P. L. Gai, *J. Chem. Sci.* **118** 37-42 (2006).
4. Can a single-reference approach provide a balanced description of ground and excited states? A comparison of the completely renormalized equation-of-motion coupled-cluster method with multireference quasidegenerate perturbation theory near a conical intersection and along a photodissociation coordinate in ammonia, S. Nangia and D. G. Truhlar, M. J. McGuire, and P. Piecuch, *J. Phys. Chem A* **109**, 11643-11646 (2005).
3. Introductory lecture: Nonadiabatic effects in chemical dynamics, A. W. Jasper, CY. Zhu, S. Nangia, and D. G. Truhlar, *Faraday Discuss.* **127**, 1-22 (2004).
2. Coherent switching with decay of mixing: An improved treatment of electronic coherence for non-Born-Oppenheimer trajectories, CY. Zhu, S. Nangia, A. W. Jasper, and D. G. Truhlar, *J. Chem. Phys.* **121**, 7658-7670 (2004).
1. Army ants algorithm for rare event sampling of delocalized nonadiabatic transitions by trajectory surface hopping and the estimation of sampling errors by the bootstrap method, S. Nangia, A. W. Jasper, T. F. Miller III, and D. G. Truhlar, *J. Chem. Phys.* **120**, 3586-3597 (2004).

PRESENTATIONS

- (Oral) Dissolution studies of mineral-water interfaces using newly developed Monte Carlo algorithm, at 237th ACS National Meeting, Salt Lake City UT (March 22-26, 2009).
- (Poster) Reaction mechanisms and dissolution rates of quartz in acidic, basic, and neutral media, at 234th ACS National Meeting, Boston MA (August 19-23, 2007).
- (Poster) Army Ants Algorithm for Surface Hopping Calculations on Chemical Systems with Coupled Electronic States," at *Computational Chemical Dynamics from Gas-Phase to Condensed-Phase Systems*, University of Minnesota, Minneapolis (October 7-9, 2004).

- (Poster) Army Ants Algorithm for Efficient Trajectory Surface Hopping, at *Non-adiabatic Effects in Chemical Dynamics*, Faraday Discussions 127, Oxford, UK (5-7 April 2004).

SERVICE

- Chair, VOICES committee – Organizer of conference for Women in Science and Engineering
- Judge, 11th Annual Environmental Chemistry Student Symposium hosted by the Center for Environmental Chemistry and Geochemistry (CECG), March 28 - 29, 2008
- Member, Graduate Women in Science (GWIS)

GRANT WRITING EXPERIENCE

- The Camille and Henry Dreyfus Foundation: Postdoctoral Program in Environmental Chemistry (2007)
- National Center for Supercomputing Applications (NCSA) at the University of Illinois, Urbana-Champaign: One year allocation on the NCSA TeraGrid, (2007–2008)

REVIEWER EXPERIENCE

Invited to review manuscripts for

- Journal of Chemical Physics
- Langmuir
- Geochimica et Cosmo. Acta
- Journal of Physical Chemistry
- Surface Science
- Journal of Vacuum Science and Technology

SUPERVISING EXPERIENCE

Supervised graduate and undergraduate students

- Christin Morrow (Graduate Student, Pennsylvania State University)
- Michael Skowronski (Undergraduate, Pennsylvania State University)
- Jill Zwickl (Undergraduate student, University of Minnesota)

REFERENCES

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