Rajiv K. Kalia

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CURRENT POSITION:	Professor
	Department of Physics and Astronomy
	Department of Chemical Engineering and Material Science
	Department of Computer Science
	University of Southern California
EDUCATION:	Ph.D., Northwestern University, 1976.

PROFESSIONAL EXPERIENCE:

2002 - Present	Professor, Joint Appointment in the Departments of Physics & Astronomy, Materials Science, and Computer Science University of Southern California
1990 - 2002	Professor, Joint Appointment in the Department of Physics & Astronomy and the Department of Computer Science Louisiana State University, Baton Rouge
2000 - 2001	Director, Biological Computation and Visualization Center Louisiana State University, Baton Rouge
1979 - 1990	Research Scientist, Argonne National Laboratory
1976 - 1979	Research Associate, Brown University

CONCURRENT POSITIONS:

2000	Visiting Professor, TU Delft, The Netherlands
1988	Visiting Scientist, IFF, Kernforschungsanlage, Jülich, Germany
1986	Visiting Professor, University of São Paulo, São Carlos, Brazil
1985	Visiting Scientist, Massachusetts Institute of Technology

AWARDS AND HONORS:

2010	USC Viterbi School of Engineering Senior Research Award
2007	Fellow of the American Physical Society
2000	FOM Fellowship, The Netherlands
1999	Recipient of the LSU Distinguished Faculty Award
1997	DARPA Sustained Excellence Award in Ultra Dense, Ultra Fast Computing Components, as a USC-LSU MURI team member
1991	Japan Society for the Promotion of Science Fellowship

RESEARCH INTERESTS

Multi-scale simulations of nano-structured materials and processes using quantum molecular dynamics (QMD), reactive molecular dynamics (RMD), and dissipative particle dynamics stimulations of hard and soft materials. Current research efforts are focused on petascale simulations of: 1) self-healing nanomaterials capable of sensing and repairing damage in harsh chemical environments and in high-temperature/high-pressure operating conditions; 2) structural and dynamic correlation in fluids confined in nanoporous materials; 3) nanoengineered energetic materials and munitions under extreme conditions; 4) shock propagation and pressure-induced structural transformations in nanocluster assemblies and self-assembled monolayers; 5) nucleation and growth of cracks, stress corrosion, and delamination at metal/ceramic, semiconductor/ceramic, and polymer/ceramic interfaces; 6) cholesterol flip-flop dynamics and barriers to small interfering RNA delivery across biomembranes; and 7) supercrystals of DNA-functionalized metal nanoparticles. Also developed and implemented fully integrated density functional, molecular dynamics, and finite element schemes on a Grid of distributed parallel supercomputers and networked virtual environment.

EDUCATIONAL PROGRAMS

Dual-degree Program

We have established a unique **dual-degree program**, in which students can obtain a Ph.D. in the physical sciences or engineering and an M.S. in computer science in five years. The program is designed to produce a new generation of computational scientists who will make innovative use of emerging information technologies to address Grand Challenge problems in their application domains. We have introduced cross-disciplinary courses in support of this dual-degree program. Efforts are underway to make the MS program in computer science accessible to students anywhere and anytime through USC's top-rated distance-education learning program.

Courses Taught

Statistical physics; mathematical physics; modern physics; condensed matter physics; computational sciences; parallel computing.

OUTREACH

We have established a special program for undergraduate students and their faculty mentors from Historically Black Colleges and Universities (HBCUs) and Minority Serving Institutions (MSIs). Groups of two students and one faculty are brought together from 12 institutions to participate in a one-week workshop on computational sciences. Students come with varying backgrounds—freshmen through seniors—and receive hands-on experience in parallel computing, including the assembly of PC nodes from off-the-shelf components, loading them with scientific and simulation software, and connecting them to a Gigabit switch. This parallel cluster is then used for algorithmic and simulation exercises in a tutorial setting. In addition to hands-on activities, the participants visit research laboratories and attend lectures on emerging trends in physical and computer sciences and engineering. Follow-on activities with participants include: (1) Bringing students back for summer research; (2) remote research experiences for students facilitated by the loan of the PCs they build at the workshop; and (3) inviting 2-3 students and 2-3 faculty mentors from the previous workshop to help run the next workshop.

RESEARCH INFRASTRUCTURE

***Local parallel computing resources*:** We established a Collaboratory for Advanced Computing and Simulations (CACS) at USC in September 2002. The CACS has 4,096-core Linux clusters, amounting to 36 million core-hours/year of dedicated computing. In addition, we have 200 million hours of computing allocation from the Department of Energy through an INCITE grant.

Collaborative immersive and interactive visualization facilities: The CACS also has: 1) a 14'×8' tiled display driven by a 26-processor Linux cluster; 2) an immersive and interactive virtual environment, ImmersaDesk; and 3) an Access Grid for remote audio and video collaboration and conferencing. The ImmersaDesk provides interactive, stereoscopic data projection. The Access Grid consists of a dedicated space with immersive audio and visualization capabilities for tutorials, lectures, meetings, conferences, and all other forms of interactions that currently require face-to-face meetings.

National and international computing resources: We have dedicated access to the IBM Blue Gene/L at Lawrence Livermore National Laboratory and IBM Blue Gene/P at Argonne National Labpratory for our SCiDAC project.

MULTIINSTITUTIONAL, MULTIDISCIPLINARY ACTIVITIES

NSF CDI-Type II: "Probing Complex Dynamics of Small Interfering RNA (siRNA) Transfection by Petascale Simulations and Network Analysis": We (Kalia, Nakano, Vashishta at USC; Grama at Purdue) are performing multimillion-atom simulations to study: (1) the effect of siRNAs on the molecular structure of lipid membranes and how structural changes affect the membrane permeability; and (2) delivery of siRNAs encapsulated in liposomes by ultrasound.

NSF—Cholesterol *Flip-flop Dynamics and Nanomechanical Response of Deformed Biomembranes: Experiments and Petascale Simulations:* In this joint experimental and computer simulation project, we (Kalia, Malmstadt, Nakano, Vashishta at USC) are investigating the nanomechanical response of phase separated liquid-ordered and liquid-disordered domains to membrane deformation and how cholesterol flip-flop dynamics between the membrane leaflets affect the mechanical response.

NSF Information Technology Research (ITR), "De Novo Hierarchical Simulations of Stress Corrosion Cracking in Materials": We are spearheading (Kalia, Nakano, Vashishta—PI) a $3.8M project with Caltech (W. Goddard and M. Ortiz) and Purdue (A. Grama) to study atomistic mechanisms of stress corrosion cracking by high-end parallel and Grid simulations that seamlessly integrate quantum mechanical simulations, molecular dynamics simulations with reactive and nonreactive force fields, accelerated dynamics, and atomistically informed continuum models.

DOE Energy Frontier Research Center on "Emerging Materials for Solar Energy Conversion and Solid State Lighting"*:* This EFRC involves collaboration between University of Southern California, University of Illinois, University of Michigan and University of Virginia. Research at the Center is focused on emerging materials for solar energy and solid-state lighting and the invention of new solar cell and LED designs based on nanostructured and organic materials.

DOE-SciDAC, **"***Hierarchical Petascale Simulation Framework for Stress Corrosion Cracking***"**: We (Kalia, Nakano, Vashishta) are leading this collaboration with Kaxiras (Harvard) G. Lu (Cal State Northridge); A. Grama (Purdue); J. Moriarty and L. Yang (Livermore); A. Voter (Los Alamos). The project focuses on scalable parallel and distributed computational framework for stress corrosion cracking.

DOE SciDAC-e, "***Performance enhancement of simulating the dynamics of photoexcitation for solar energy conversion***": In collaboration with Maryland (J. Hollingsworth), LLNL (D. Quinlan), and Utah (M. Hall), we (R. Lucas—PI, J. Chame, P. Diniz, R. K. Kalia, A. Nakano, P. Vashishta) enhance the performance of our petascale nonadiabatic quantum molecular dynamics simulation codes to study photoexcitation dynamics for solar energy applications.

PROPOSALS FUNDED

1. Molecular mechanisms of spore killing by corrosive and detonation product gases: Reactive molecular dynamics coupled with graph-theoretic methods
   P. Vashishta, R. K. Kalia, A. Nakano
   DoD DTRA program: $750,000 for 5 years

2. Probing complex dynamics of small interfering RNA transfection by petascale simulations
   P. Vashishta, R. K. Kalia, A. Nakano (USC); A. Grama (Purdue University
   National Science Foundation, Collaborative Research: CDI-Type II, $1,080,000

3. Synthesis, characterization, and multiscale simulations of low-cost high density insensitive high performance energetic composite molecular systems for future Navy adaptive weapon requirements
   P. Vashishta-PI, R. K. Kalia, A. Nakano, K. Christie (USC); S. Stewart (UIUC); Y. Gupta (WSU), ONR, $3,175,000

4. Multimillion-to-billion atom simulations of nanoscale systems
   P. Vashishta, R. K. Kalia, A. Nakano
   Department of Energy, BES program: $540,000 for 3 years

5. Petascale hierarchical simulations of biopolymer translocation through silicon nitride and silica nanopores and nanofluidic channels
   P. Vashishta, R. K. Kalia, A. Nakano, M. Hall, jointly with University of California, Santa Barbara
   National Science Foundation, PetaApps Program, CACS portion: $1,575,000 for 5 years

6. Cholesterol flip-flop dynamics and nanomechanical response of deformed biomembranes: Experiments and petascale simulations
   N. Malmstadt, R. K. Kalia, A. Nakano, P. Vashishta
   National Science Foundation, $200,000

7. Petascale simulations of self-healing nanomaterials
   Rajiv K. Kalia-PI and Aiichiro Nakano
   DOE INCITE program, 2014-17; 600 million hours of computing allocation on MIRA at Argonne National Laboratory

8. GPU-accelerated computing platform for simulation and visualization of insensitive nanoenergetic materials
   DoD-DURIP, $200,000

PROPOSALS PENDING

1. Predictive Theory/Simulation to Guide the Design and Synthesis of Novel Stimuli-Responsive Metal Organic Frameworks (MOFs) and Embedding of Metalloid Clusters inside MOF Cavities by Atomic Deposition using Property-Directing Ligands
   DoD-MURI, $7.5 Million for 5 Years

2. Metascalable Quantum and Reactive Molecular Dynamics Simulation Algorithms for Million-Core Architectures and their Applications to Stacked Atomic-Layer Heterostructures
   DoD-HASI, $2.0 Million for 4 years

3. Bactericidal Synthetic Nanopillars
   NSF: $450,000 for 3 years

CONFERENCE ACTIVITIES

- APS Meeting Symposium Co-organizer: "50 Years of MD"
  March 2-5, 2015, San Antonio, TX

- "Vashishta Festschrift"
  August 29, 2014, University of Southern California

- Co-organizer, "Meeting on Energetic Materials"
  December 3-4, 2012, Terranea Resort in Greater Los Angeles, CA.

- Co-organizer, "Materials Genome: Simulations, Synthesis, Characterization and Manufacturing"
  April 4–6, 2012, Terranea Resort in Greater Los Angeles, CA.

- Co-organizer, European Materials Research Society Symposium on "*DNA Directed Programmable Self-assembly of Nanoparticles into Metamaterials for Energy and other Applications*", Strasbourg, France, May 14-18, 2012.

- Co-organizer, "*Materials for Energy Applications: Experiment, Modeling and Simulations*"
  March 30–April 1, 2011, Terranea Resort in Greater Los Angeles, CA.

- Co-organizer, "*Emerging Trends in Materials Simulations and Experiments*"
  March 24-26, 2010, Terranea Resort in Greater Los Angeles, CA.

- Organizer of the "*Computational Science Workshop for Underrepresented Groups*"
  June 21-29, 2009, University of Southern California, Los Angeles, CA.

- Organizer of the "*Computational Science Workshop for Underrepresented Groups*"
  May 18-25, 2008, University of Southern California, Los Angeles, CA.

- Organizer of the "*Computational Science Workshop for Underrepresented Groups*"
  January 3-10, 2007, University of Southern California, Los Angeles, CA.

- International Workshop on "*Neutrons and Grand Challenges of Nanoscience, Energy Research, and Computation*"
  November 16-18, 2006, Xi'an, China.

- SciDAC Kickoff Meeting on "*Stress Corrosion Cracking*"
  November 11, 2006, University of Southern California, Los Angeles, CA.

- Organizer of the "*Computational Science Workshop for Underrepresented Groups*",
  January 5-11, 2006, University of Southern California, Los Angeles, CA.

- Organizer of the USC-CALTECH meeting on "*High Strain Rate Deformation and Shock Phenomena*", October 6 & 7, 2005, University of Southern California, Los Angeles, CA.

- Organizer of the "*Computational Science Workshop for Underrepresented Groups*",
  January 5-11, 2005, University of Southern California, Los Angeles, CA.

- Co-organizer of a Symposium at the "*International Conference on Fracture*"
  March 20-25, 2005, Turin, Italy.

- Conference on "*Computational and Experimental Challenges in Physical, Chemical and Biological Systems*", August 20-21, 2004, Univ. of Southern California, Los Angeles, CA.

- Co-organizer of the International Conference on "*Dynamics of Disordered Materials on the Nanometer Scale*", February 23-27, 2004, Hanoi, Vietnam.

- Co-organizer of the "*US-Vietnam Symposium*", March 1-2, 2004, Hanoi, Vietnam.

- Organizer of the "*Computational Science Workshop for Underrepresented Groups*",
  January 5-10, 2004, University of Southern California, Los Angeles, CA.

- Co-organizer of the Mardi Gras 2003 Conference on "*Grid Computing and Simulation at the Nano-Bio Interface*", February 27-March 1, 2003, Louisiana State University, Baton Rouge, LA.
- Organizer of the "*Computational Science Workshop for Underrepresented Groups*", January 5-11, 2003, Louisiana State University, Baton Rouge, LA.
- Co-organizer of the Mardi Gras 2002 Conference on "*Nanotechnology at the Interface of Information Technology*", February 7-9, 2002, Louisiana State University, Baton Rouge, LA.
- Co-organizer of the "*Computational Science Workshop for Underrepresented Groups*", January 4-10, 2002, Louisiana State University, Baton Rouge, LA.
- Co-organizer of the Mardi Gras 2001 Conference on "*Multiscale Simulation, Theoretical, and Experimental Approaches to Deformation, Friction, Fatigue, and Fracture*", February 22-24, 2001, Baton Rouge, LA.
- Co-organizer of the International Conference on "*Multiscale Materials Phenomena in Harsh Environments*", June 19-24, 2000, Limassol, Cyprus.
- Co-organizer of the Mardi Gras 2000 Conference on "*Material Design: Experimental and Computational Challenges*", March 2-4, 2000, Baton Rouge, LA.
- Co-organizer of the Workshop on "*Parallel Algorithms, Computational Efficiency and Multiscale Materials Simulations*", April 2-3, 1999, New Orleans, LA.
- Co-organizer of the International Conference on "*Thermo-Mechanical and Electrical Properties of High-Temperature Materials*", Maui, January 6-11, 1999.
- Advisory Committee of the Workshop on "*Advanced Materials for Extreme Environments: New Experimental Opportunities in Neutron Scattering,*" Argonne National Laboratory, Argonne, IL, September 10 - 12, 1998.
- Co-organizer, Materials Research Society Symposium on "*Computational and Mathematical Models of Microstructural Evolution,*" San Francisco, CA, April 13-17, 1998.
- Co-organizer, APS 1998 March Meeting Focused Session on "*Materials Theory and Simulation.*"
- Co-organizer, International Conference on "*Materials and Microsystems for Extreme Environments: Experimental and Computational Challenges,*" February 19-21, 1998, Baton Rouge, LA.
- Co-organizer, International Conference on "*Computer-Aided Design of High-Temperature Materials,*" July 30 - August 2, 1997, Santa Fe, NM.
- Co-organizer, International Conference on "*Multiscale Phenomena in Science and Engineering,*" February 7-9, 1997, Baton Rouge, LA.
- Co-organizer, International Conference on "*Experimental and Simulation Challenges in Nanostructured Materials,*" February 15-17, 1996, Baton Rouge, LA.
- Co-organizer, Materials Research Society Symposium on "*Materials Theory, Simulations, and Parallel Algorithms,*" November 27 - December 31, 1995, Boston, MA.
- Co-organizer, International Conference on "*High Performance Computing Technologies and Scientific Applications,*" February 23-25, 1995, Baton Rouge, LA.
- Co-organizer, International Conference on "*Teraflop Computing and New Grand Challenge Applications,*" February 10-12, 1994, Baton Rouge, LA.
- Chairman, International Conference on "*Concurrent Computing in the Physical Sciences,*" February 18-20, 1993, Baton Rouge, LA.
- Co-organizer, "*Parallel Adventure*" Workshop, August 3-7, 1992, Baton Rouge, LA.
- Co-organizer, Workshop on "*Undergraduate and Graduate Education in Computational Sciences,*" April 29-30, 1991, Baton Rouge, LA.

- Co-organizer, Symposium on "*Concurrent Computing in the 90s*," August 17, 1990, Baton Rouge, LA.
- Director, Symposium on "*Highlights in Condensed Matter Physics*," International Center for Theoretical Physics, August 1-3, 1989, Trieste, Italy.
- Conference Organizer, "*9th Midwest Solid State Theory Symposium*," November 2-3, 1981, Argonne National Laboratory, Argonne, IL.

PUBLICATIONS

Books

- *Melting, Localization and Chaos*
  Eds: R. K. Kalia and P. Vashishta, Elsevier North-Holland, New York (1982).
- *Condensed Matter Theories, Vol. 2*
  Eds: P. Vashishta, R. K. Kalia, and R. Bishop, Plenum, New York (1987).
- *Correlations in Electronic and Atomic Fluids*
  Eds: P. Jena, R. K. Kalia, P. Vashishta, and M. P. Tosi, World Scientific, Singapore, (1990).
- *High Performance Computing and its Applications in the Physical Sciences*
  Eds. D. A. Browne, J. Callaway, J. P. Draayer, R. W. Haymaker, R. K. Kalia, J. E. Tohline, and P. Vashishta, (World Scientific, Singapore,1994).
- *Teraflop Computing and Grand Challenge Applications*
  Eds. R. K. Kalia and P. Vashishta, Nova Science Publishers, NY (1995).
- *Materials Theory, Simulations, and Parallel Algorithms*
  Eds. E. Kaxiras, J. Joannopoulos, P. Vashishta, and R. K. Kalia, MRS symposium proceedings (1996).
- *Computational and Mathematical Models of Microstructural Evolution*
  Eds. J. Bullard, L-Q. Chen, R. K. Kalia, and M. Stoneham, MRS proceedings (1998).
- *Computer-Aided Design of High-Temperature Materials*
  Eds. A. Pechenik, R. K. Kalia, and P. Vashishta, Oxford University Press, Oxford (1999).

Research Publications

1. On the Dynamic Form Factor of an Electron Liquid
   R. K. Kalia and G. Mukhopadhyay, Solid State Commun. **15**, 1243 (1974).

2. Dynamic Structure Factor of an Electron Liquid
   G. Mukhopadhyay, R. K. Kalia, and K. S. Singwi, Phys. Rev. Lett. **15**, 950 (1974).

3. Surface Energy of Electron-Hole Liquid in Germanium at Zero and Finite <111> Uniaxial Stress
   P. Vashishta, R. K. Kalia, and K. S. Singwi, Solid State Commun. **19**, 935 (1976).

4. Surface Properties of Electron-Hole Drops in Germanium
   P. Vashishta, R. K. Kalia, and K. S. Singwi, in Physics of Highly Excited States in Solids, eds. M. Ueta and Y. Nishina, Springer-Verlag, vol. **57**, 1976, p. 187.

5. Sign Reversals of Charge on Electron-Hole Drops
   R. K. Kalia and P. Vashishta, Solid State Commun. **24**, 171 (1977).

6. Exchange Instabilities in an n-type Silicon Inversion Layer
   R. K. Kalia and J. J. Quinn, Phys. Rev. **B 17**, 1383 (1978).

7. Surface Structure of Electron Hole Drops in Germanium and Silicon
   R. K. Kalia and P. Vashishta, Phys. Rev. **B 17**, 2655 (1978).

8. Temperature Dependence of Many-Body Effects in Inversion Layers
   R. K. Kalia, S. DasSarma, M. Nakayama, and J. J. Quinn, Phys. Rev. **B 18**, 5564 (1978).

9. Stress and Temperature Dependence of Subband Structure in (100)-Silicon Inversion Layer
   S. DasSarma, R. K. Kalia, M. Nakayama, and J. J. Quinn, Phys. Rev. **B 19**, 6397 (1979).

10. Temperature Dependence of Subband Energies in Semiconducting Surface Inversion Layers: Exchange and Correlation Effects
R. K. Kalia, S. DasSarma, M. Nakayama, and J. J. Quinn, Proc. <u>14th International Conference on the Physics of Semiconductors</u>, ed. B. L. H. Wilson, Institute of Physics (Bristol and London), 1979, vol. **43**, p. 1251.

11. Self-Consistent Surface Calculations of Electron-Hole Drops in Gallium Phosphide
R. K. Kalia and P. Vashishta, Solid State Commun. **34**, 121 (1980).

12. A Simplified Treatment of Exchange and Correlation in Semiconducting Surface Inversion Layers
R. K. Kalia, G. Kawamoto, J. J. Quinn, and S. C. Ying, Solid State Commun. **34**, 423 (1980).

13. Final-State Interaction and Inter-Subband Spectroscopy in Silicon Inversion Layers
S. DasSarma, R. K. Kalia, M. Nakayama, and J. J. Quinn, Phys. Rev. **B 24**, 7181 (1981).

14. Evidence for a Valley-Occupancy Transition in Si Inversion Layers at Low Electron Densities
T. Cole, B. D. McCombe, J. J. Quinn, and R. K. Kalia, Phys. Rev. Lett. **46**, 1096 (1981).

15. Melting of a Two-Dimensional Electron Lattice
R. K. Kalia, P. Vashishta, and S. W. de Leeuw, Phys. Rev. **B 23**, 4794 (1981).

16. Interfacial Colloidal Crystals and Melting Transition
R. K. Kalia and P. Vashishta, J. Phys. **C 14**, L643 (l981).

17. On the Oscillatory Behavior of Velocity Auto-Correlation Function of a 2D Electron Liquid
R. K. Kalia, P. Vashishta, S. W. de Leeuw, and A. Rahman, J. Phys. **C 14**, L991 (l981).

18. Melting and Nucleation of a Two-Dimensional Electron Solid
R. K. Kalia and P. Vashishta, in <u>Physics of Intercalation Compounds</u>, eds. L. Pietronero and E. T. Tosatti, Springer Verlag, vol. **38**, 1981, p. 244.

19. Melting and Freezing in Two Dimensions: A Molecular Dynamics Study
P. Vashishta and R. K. Kalia, in <u>Melting, Localization and Chaos</u>, eds. R. K. Kalia and P. Vashishta, (North-Holland, NY), l982, p. 43.

20. Molecular Dynamics Study of 2-D Melting: Long Range Potentials
R. K. Kalia and P. Vashishta, in <u>Nonlinear Phenomena at Phase Transitions and Instabilities</u>, ed. T. Riste, Plenum, p. 425, 1982.

21. Orientational Order-Disorder Transition on a Surface
R. K. Kalia, S. D. Mahanti, and P. Vashishta, Phys. Rev. Lett. **49**, 676 (1982).

22. Universal Behavior of Exchange-Correlation Energy in Electron-Hole Liquid
P. Vashishta and R. K. Kalia, Phys. Rev. **B 25**, 6492 (1982).

23. Melting, Freezing and Order-Disorder Transition in Two Dimensions
P. Vashishta and R. K. Kalia, in Proc. of <u>6th Pan American Workshop on Condensed Matter Theories</u>, Washington Univ., St. Louis, MO, Sept. 20-Oct. 1, 1982. Ed. J. W. Clark.

24. Electron-Hole Liquid: Theory
P. Vashishta, R. K. Kalia, and K. S. Singwi, in <u>Electron-Hole Droplets in Semiconductors</u>, eds. C. D. Jeffries and L. V. Keldysh, (North-Holland, NY), l983, p. 1.

25. Ground State Properties, Thermodynamics and Systematics of Electron-Hole Liquid in Ge and Si Under Varying Uniaxial Stress
G. Vignale, R. K. Kalia, P. Vashishta, and K. S. Singwi, J. Phys. **C 16**, 699 (1983).

26. Electrons on Corrugated Surfaces
    R. K. Kalia, P. Vashishta, S. D. Mahanti, and J. J. Quinn, J. Phys. **C 16**, L491 (1983).

27. Comment on a *Variational Approach to the Ground State of Electron-Hole Liquid*
    P. Vashishta, R. K. Kalia, and K. S. Singwi, Phys. Rev. Lett. **50**, 203 (1983).

28. Melting and Crystallization on Corrugated Surfaces
    P. Vashishta, R. K. Kalia, and J. J. Quinn, J. Phys. **C 16**, L405 (1983).

29. The Ground State of Excitonic Molecules by the Green's Function Monte Carlo (GFMC) Method
    M. A Lee, P. Vashishta, and R. K. Kalia, Phys. Rev. Lett. **51**, 2422 (1983).

30. Electrons on Sinusoidal Corrugations - A Tricritical Melting Point
    P. Vashishta, R. K. Kalia, and J. J. Quinn, Proc. Int. Conf. <u>Recent Progress on Many-Body Theories</u>, Altenberg, W. Germany, Aug. 29-Sept. 3, 1983.

31. Topological Defects and Melting of Wigner Solid on Corrugated Surfaces
    P. Vashishta, R. K. Kalia, and J. J. Quinn, Surf. Sci. **142**, 120 (1984).

32. Melting of Electrons on Corrugated Surfaces - Structural and Dynamical Properties in Liquid and Solid Phases
    P. Vashishta, R. K. Kalia, and J. J. Quinn, <u>Lecture Notes in Physics</u>, eds. H. Kümmel and M. L. Ristig, Springer-Verlag, vol. **198**, p. 235, 1984.

33. Binding Energy of Positively Charged Acceptors in Germanium - A Green's Function Monte Carlo Calculation
    R. K. Kalia, P. Vashishta, and M. A. Lee, Solid State Commun. **52**, 873 (1984).

34. Microscopic Structure of Two-Dimensional Electron Glass
    R. K. Kalia and P. Vashishta, Materials Science Forum **4**, 99 (1985).

35. Quantum Simulation of Small Electron-Hole Complexes
    M. A. Lee, R. K. Kalia, and P. Vashishta, Materials Science Forum **4**, 165 (1985).

36. Topological Disorder and Bi-Level States in the 2-D Electron Glass
    R. K. Kalia and P. Vashishta, Solid State Commun. **55**, 843 (1985).

37. Fractal Dimensionality of Brownian Motion in Two Dimensions
    R. K. Kalia, S. W. de Leeuw, and P. Vashishta, J. Phys. **C 18**, L905 (1985).

38. Lennard-Jones Molecules on a Two-Dimensional Lattice: A Model Anisotropic XY System
    S. Tang, S. D. Mahanti, and R. K. Kalia, Phys. Rev. **B 32**, 3148 (1985).

39. On Isosets of Brownian Motion
    S. W. de Leeuw, R. K. Kalia, and P. Vashishta, Solid State Commun. **57,** 749 (1986).

40. Fractal Dimensionalities of Ionic Trails and Isosets in Superionic Conductors
    P. Vashishta, I. Ebbsjö, R. K. Kalia, and S. W. de Leeuw, Solid State Commun. **59**, 873 (1986).

41. Fractal Dimensionalities of Brownian Trajectories and Brown Isosets in Superionic and Molten Ag_2S
    P. Vashishta, I. Ebbsjö, R. K. Kalia, and S. W. de Leeuw, <u>Proc. V Int. Symp. on Molten Salts</u>, Las Vegas, NV, October 14-18, 1985, The Electrochemical Society, Inc., Pennington, NJ, 1986, Vol. **86-l**, p. 49.

42. Ferroelastic Phase Transition in Two-Dimensional Molecular Solids
    S. Tang, S. D. Mahanti, and R. K. Kalia, Phys. Rev. Lett. **56**, 484 (1986).

43. Fractal Behavior of Isosets and Trails in Superionic Conductors
    P. Vashishta, I. Ebbsjö, R. K. Kalia, and S. W. de Leeuw, Solid State Ionics **18 & 19**, 169 (1986).

44. New Aspects of Variable-Range Hopping in Finite One-Dimensional Wires
R. A. Serota, R. K. Kalia, and P. A. Lee, Phys. Rev. **B 33**, 8441 (1986).

45. Fractal Behavior of Single-Particles Trajectories and Isosets in Isotropic and Anisotropic Fluids
R. K. Kalia, P. Vashishta, and S. W. de Leeuw, <u>Condensed Matter Theories</u>, ed. F. B. Malik, (Plenum, NY), 1986, vol. 1, p. 285.

46. Tricritical Behavior in the Ferromagnetic Superconductor $ErRh_4B_4$
G. W. Crabtree, R. K. Kalia, D. G. Hinks, F. Behroozi, and M. Tachiki, J. Magn. Mater. **54-57**, 703 (1986).

47. Molecular Dynamics Study of a Two-Dimensional System with Screened Coulomb Interactions
H. Cheng, P. Dutta, D. E. Ellis, and R. K. Kalia, J. Chem. Phys. **85**, 2232 (1986).

48. Hopping Magnetoconduction and the Random Structure in Quasi One-Dimensional Inversion Layers
R. K. Kalia, W. Xue, and P. A. Lee, Phys. Rev. Lett. **57**, 1615 (1986).

49. Fragmentation of Silicon Microclusters: A Molecular Dynamics Study
B. P. Feuston, R. K. Kalia, and P. Vashishta, Phys. Rev. **B 35**, 6222 (1987).

50. Fragmentation and Structure of Silicon Microclusters
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M. Kunaseth, D. F. Richards, J. N. Glosli, R. K. Kalia, A. Nakano, and P. Vashishta *Proceedings of International Workshop on Parallel and Distributed Scientific and Engineering Computing* (2013).

359. Collective oxidation behavior of aluminum nanoparticle aggregate
A. Shekhar, W. Wang, R. Clark, R. K. Kalia, A. Nakano, and P. Vashishta *Applied Physics Letters* **102**, 221904: 1-4 (2013).

360. Bonding and structure of ceramic-ceramic interfaces
K. Shimamura, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Physical Review Letters **111**, 066103: 1-5 (2013).

361. Analysis of scalable data-privatization threading algorithms for hybrid MPI/OpenMP parallelization of molecular dynamics
Manaschai Kunaseth, David F. Richards, James N. Glosli, Rajiv K. Kalia, Aiichiro Nakano, Priya Vashishta
J. Supercomput. **66**, 406–430 (2013).

362. Size effect on the oxidation of aluminum nanoparticle: Multimillion-atom reactive molecular dynamics simulations
Ying Li, Rajiv K. Kalia, Aiichiro Nakano, and Priya Vashishta
J. Appl. Phys. **114**, 134312 (2013).

363. Shock loading on AlN ceramics: A large-scale molecular dynamics study
Paulo S. Branicio, Aiichiro Nakano, Rajiv K. Kalia, Priya Vashishta
International Journal of Plasticity **51,** 122–131 (2013).

364. Scalability study of molecular dynamics simulation on Godson-T many-core architecture
Liu Penga, Guangming Tan, Rajiv K. Kalia, Aiichiro Nakano, Priya Vashisht, Dongrui Fan, Hao Zhang, Fenglong Song
J. Parallel Distrib. Comput. **73**, 1469–1482 (2013).

365. Rapid hydrogen production from water using aluminum nanoclusters: a quantum molecular dynamics simulation study
P. Vashishta, F. Shimojo, S. Ohmura, K. Shimamura, W. Mou, R. K. Kalia, and Aiichiro Nakano
Solid State Ionics **262**, 908-910 (2014).

366. A divide-conquer-recombine algorithmic paradigm for large spatiotemporal quantum molecular dynamics simulations
F. Shimojo, S. Hattori, R. K. Kalia, M. Kunaseth, W. Mou, A. Nakano, K. Nomura, S. Ohmura, P. Rajak, K. Shimamura, and P. Vashishta
Journal of Chemical Physics **140**, 18A529: 1-14 (2014).

367. Small Interfering RNA induces liquid-to-ripple phase transformation in a phospholipid membrane
A. Choubey, K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letters **105**, 113702: 1-4 (2014).

368. Universal stretched exponential relaxation in nanoconfined water
A. Shekhar, R. K. Kalia, A. Nakano, P. Vashishta, C. K. Alm, and A. Malthe-Sorenssen
Applied Physics Letters **105**, 161907: 1-4 (2014).

369. Multistage reaction pathways in detonating high explosives
Y. Li, R. K. Kalia, A. Nakano, K. Nomura, and P. Vashishta
Applied Physics Letters **105**, 204103: 1-5 (2014).

370. Hydrogen-on-demand using metallic alloy nanoparticles in water
K. Shimamura, F. Shimojo, R. K. Kalia, A. Nakano, K. Nomura, and P. Vashishta
Nano Letters **14**, 4090-4096 (2014).

371. Nanoindentation of NiAl and Ni3Al crystals on (100), (110), and (111) surfaces: a molecular dynamics study
R. Seymour, A. Hemeryck, K. Nomura, W. Wang, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letter **104**, 141904: 1-4 (2014).

372. A divide-conquer-recombine algorithmic paradigm for large spatiotemporal quantum molecular dynamics simulations
F. Shimojo, S. Hattori, R. K. Kalia, M. Kunaseth, W. Mou, A. Nakano, K. Nomura, S. Ohmura, P. Rajak, K. Shimamura, and P. Vashishta
Journal of Chemical Physics **140**, 18A529: 1-14 (2014).

INVITED TALKS

- Melting of a Two-Dimensional Electron Solid
  <u>Annual Meeting of the American Physical Society</u>, Phoenix, AZ, March 1981.

- Molecular Dynamics Study of 2D Melting: Long Range Potentials
  NATO Advanced Study Institute on <u>Nonlinear Phenomena at Phase Transitions and Instabilities</u>, Geilo, Norway, March 29-April 9, 1981.

- Melting and Nucleation of a Two-Dimensional Coulomb Solid
  International Conference on <u>Physics of Intercalation Compounds</u>, I.C.T.P. Trieste, Italy, July 6-10, 1981.

- Melting and Freezing in Two Dimensions: A Molecular Dynamics Study
  <u>9th Midwest Solid State Theory Symposium</u>, Argonne National Laboratory, Argonne, IL. Nov. 2-3, 1981.

- Electrons on Smooth and Corrugated Surfaces
  <u>10th Midwest Solid State Theory Symposium</u>, Michigan State University, East Lansing, MI, Oct. 8-9, 1982.

- Microscopic Structure of Electron Glass in Two Dimensions
  <u>12th Midwest Solid State Theory Symposium</u>, University of Minnesota, October 1984.

- Fractal Dimensions of Brown Trails and Isosets in Superionic and Molten Ag_2I
  <u>Electrochemical Society Meeting</u>, Las Vegas, NV, October 14-18, 1985.

- Monte Carlo and Molecular Dynamics Simulations of Condensed Matter Systems
  Workshop on the <u>Electronic Structure of Defects</u>, Argonne National Laboratory, Argonne, IL, June 2-13, 1986.

- Random Resistance Fluctuations in 1D MOSFETs
  Summer Institute in Theoretical Physics, Workshop on the <u>Physics of Artificially Structured Materials,</u> Queen's University, Canada, July 1986.

- Molecular Dynamics Simulations of Classical and Quantum Systems
  Universidade de São Paulo, São Carlos, Brazil, September 1986.

- Computer Simulations in Condensed Matter Physics
  Universidade Federal de Ceara, Forta Leza, Brazil, September 1986.

- Computer Experiments on Classical Systems
  Fundacao Universidade de Amazonas, Manaus, Brazil, September 1986.

- Conductance Fluctuations in 1D MOSFETs
  Universidade Federal de São Carlos, São Carlos, Brazil, October 1986.

- Simulated Annealing Approach to Density Functional and Other Optimization Problems in Condensed Matter
  Canadian Association of Physicists Congress, June 15-17, 1987.

- Nature of Gigantic Resistance Fluctuations in 1D MOSFETs
  11th Int. Workshop on <u>Condensed Matter Theory</u>, Oulu, Finland, July 27-August 1, 1987.

- Computer Simulation of Classical and Quantum Systems
  Int. Adv. School on Statistical Physics, Chandigarh, India, Sept. 28-Oct. 9, 1987.

- Structural Correlations and Phonon Density of States in a-$GeSe_2$
  IFF in Kernforschungsanlage, Jülich, West Germany, Nov. 1987.

- Computer Simulation of Systems with Long-Range Interactions
  CECAM Workshop in Paris, France, January 11-22, 1988.

- Electron Bubbles in Helium Gas - A Quantum Molecular Dynamics Simulation
  XII Int. Workshop on <u>Condensed Matter Theories</u>, Taxco, Mexico, August 14-20, 1988.

- Quantum Molecular Dynamics Simulations
  CECAM Meeting on <u>Computational Problems of Glasses and Networks</u>, Amersfoort, The Netherlands, Sept. 10-14, 1988.

- Quantum Molecular Dynamics Simulation of Electron Self-Trapping in Helium
  "Many-Body Encounter in Minnesota," University of Minnesota, Minneapolis, May 12-13, 1989.

- Quantum Molecular Dynamics Simulation of Electron Mobility in a Dense Helium Gas
  International Workshop on Condensed Matter Theories," Campos dõ Jordão, Brazil, August 7-12, 1989.

- Simulation of Electron Transport in Disordered Systems Using Quantum Molecular Dynamics Technique
  XXIV Yamada Conference on "Strongly Coupled Plasma Physics," Lake Yamanaka, Japan, August 29-September 2, 1989.

- Behavior of Excess Electrons in Disordered Media Using Quantum Molecular Dynamics Simulation
  17th Midwest Solid State Theory Symposium, Indiana University, Bloomington, IN, October 9-10, 1989.

- Electron Transport in Disordered Systems - A Quantum Molecular Dynamics Simulation
  Annual Meeting of the American Physical Society, Anaheim, CA, March 12-16, 1990.

- Electron Transport in Amorphous Materials - A Quantum Molecular Dynamics Study
  Fortieth Annual American Crystallographic Association Meeting, New Orleans, LA, April 8-13, 1990.

- Materials Simulations using Quantum Molecular Dynamics Technique
  University of Tokyo, June 21, 1991.

- Simulation of Mixed Classical-Quantum Systems
  NEC Corporation, Tsukuba, Japan, July 19, 1991.

- Quantum Molecular Dynamics Simulation of Electron Transport in Devices
  Okayama University, Japan, July 30, 1991.

- Simulation of Classical and Quantum Systems
  Niigata University, Japan, August 1, 1991.

- Materials Simulations using Quantum Molecular Dynamics Technique
  Tohoku University, Japan, August 20, 1991.

- Multiple-time-step Molecular Dynamics Simulations on Distributed Memory MIMD Machines
  XIth Parallel Circus, Minnesota Supercomputer Institute, Minneapolis, MN, April 24-25,1992.

- Concurrent Classical and Quantum Simulations
  AFOSR Workshop on Parallel Computing in Chemistry, Washington, DC, October 25-29, 1992.

- Molecular Dynamics Simulations on Parallel Architectures
  XII SLAFES, Pichidangui, Chile, November 22-28, 1992.

- Atomistic Simulations on Parallel Architectures
  Sanibel Symposia, St. Augustine, FL, March 13-20, 1993.

- Atomistic Simulations of Condensed Phase Materials on Parallel Architectures
  High Energy Density Matter Conference, Woods Hole, MA. June 6-8, 1993.

- Structural Transformations in Glasses
  University of Amsterdam, The Netherlands, July 16, 1993.

- Large-Scale Materials Simulations on Parallel Architectures
  Symposium at Brown University, Providence, RI, September 3-4, 1993.

- Probing Amorphous Materials with Computer Experiments on Parallel Architectures
  Battelle Pacific Northwest Laboratory, Richmond, WA, November 9, 1993.

- Computer Simulation of Porous Glasses on Parallel Architectures
  1994 Simulation Multiconference, San Diego, CA, April 10-15, 1994.

- Morphology of Pores and Fracture Surfaces in Porous Silica - Multimillion Particle Molecular-Dynamics Simulations
  XVIII Int. Workshop on Condensed Matter Theories, Valencia, Spain, June 6-10, 1994.

- Massively Parallel Simulations of Nanostructured Materials
  Texas A&M University, College Station, TX.

- Multiresolution Molecular Dynamics Simulations of Real Materials Using Parallel Architectures
  Livermore National Laboratory, CA.

- Fracture and Sintering of Ceramic Materials by Parallel Molecular Dynamics
  High Performance Computational Chemistry Workshop, Pleasanton, CA.

- Large Scale Molecular Dynamics Simulation of High Temperature Ceramics
  XIX International Workshop on Condensed Matter Theories, Caracas, Venezuela.

- Studies of Nanoclusters and Amorphous Materials by Parallel Molecular Dynamics Simulations
  Annual Meeting of the American Ceramic Society, Cincinnati, OH.

- Multimillion Atom Molecular Dynamics Experiments on Parallel Architectures
  1995 Simulation Multiconference, The Society of Computer Simulation, Phoenix, AZ.

- Parallel Molecular-Dynamics Simulation of Amorphous Materials
  8th Annual Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, Univ. of Georgia, Athens, GA.

- Multimillion Particle Molecular-Dynamics Simulations for Amorphous Materials on Parallel Architectures
  Los Alamos National Laboratory, Los Alamos, NM.

- Structure, Fracture and Sintering of Silicon Nitride by Parallel Molecular Dynamics
  AFOSR Contractors' Conference, Washington, DC.

- Dynamics of Fracture in Nanophase Silicon Nitride: Million Atom Molecular-Dynamics Simulations on Parallel Machines
  AFOSR Meeting in Boulder, CO.

- Structure, Mechanical Properties, and Fracture in Nanophase Silicon Nitride: Million Atom Molecular Dynamics Simulations on Parallel Computers
  TMS Meeting, Orlando, FL.

- Morphology of Pores and Interfaces and Dynamic Fracture in Nanophase Silicon Nitride
  IMRC Meeting in Cancun, Mexico.

- Molecular-Dynamics Simulations of Nanostructured Materials
  Inelastic Nuclear Resonant Scattering Workshop, Argonne, IL.

- Massively Parallel Atomistic Simulations of Dynamic Fracture in Nanophase Materials
  Niigata Univ., Japan.

- Multimillion Atom Molecular Dynamics Simulations of Nanophase Materials on Massively Parallel Computers
  Niigata Univ., Japan.

- Multimillion Atom Molecular Dynamics Simulations of Nanophase Materials on Massively Parallel Computers
  Institute for Solid State Physics, Univ. of Tokyo.

- MD Simulation of Fracture
  Gordon Research Conference, La Barga, Italy.

- Dynamic Fracture in Nanophase Ceramics: Multimillion Atom Molecular Dynamics Simulations on Parallel Computers
  Saclay, France.

- Large Scale Simulations of High Temperature Structural Materials on Massively Parallel Computers
  DoD Challenge Meeting, Houston, TX.

- Crack Propagation and Fracture in Nanostructured Ceramics: Multimillion Atom Parallel Molecular Dynamics Simulations
  WCTCC 98, Pacific National Northwest Laboratory, Richmond, WA, June 21-23, 1998.

- Multimillion Atom Molecular Dynamics Simulations of High Temperature Ceramics
  International Conference on "New Developments in High Temperature Ceramics," Istanbul, Turkey.

- Structure and Dynamic Fracture in Nanophase Silicon Nitride and Silicon Carbide: Multimillion Atom Molecular Dynamics Simulations on Massively Parallel ComputersWorkshop on *Advanced Materials for Extreme Environments: New Experimental Opportunities in Neutron Scattering*," Argonne National Laboratory, Illinois, September 11-12, 1998.

- Grand Challenge Materials Simulations: Multimillion Atom Molecular Dynamics Simulations on Parallel Computers, SSI Collaboration Meeting, Jefferson Laboratory, Newport News, Virginia, January 20-22, 1999.

- Massively Parallel Atomistic Simulations of Nanostructured Materials, Physics Department Colloquium, Auburn University, Auburn, Alabama, February 24-25, 1999.

- Designing Novel Materials on Parallel Computers, Links for Success, The 1999 Annual Board of Regents Louisiana NSF EPSCoR Conference, Pennington Biomedical Research Conference Center, Baton Rouge, Louisiana, April 13-14, 1999.

- Computational Assisted Development of High Temperature Structural Materials, Ninth Annual DoD High Performance Computing Modernization Program Users Group Conference, Monterey, California, June 7-10, 1999.

- Multimillion Atom Molecular Dynamics Simulations of Nanostructured Materials on Parallel Machines, ACS Annual Meeting in New Orleans, August 22-26, 1999.

- Multimillion Atom Molecular Dynamics Simulations of Nanostructured Materials on Parallel Machines, International Materials Research Congress, Symposium: Theory and Computer Simulation of Materials, Cancun, Mexico, August 29 - September 2, 1999.

- Massively Parallel Materials Simulations, Colloquium in the Department of Chemical Engineering, Univ. of Cincinnati, October 21, 1999.

- Multiscale Simulations of Nanostructred Materials on Massively Parallel Compters
  CERCA, Montreal, Canada, December 8, 1999.

- Multiscale Simulations of Nanostructred Materials on Massively Parallel Compters
  Steacie Institure for Molecular Sciences, National Research, Council of Canada, Ottowa, Canada, December 10, 1999.

- Parallel Multiscale Simulations of Nanostructured Materials
  CSW 2000 EPOCHAL TSUKUBA International Congress Center, March 13-15, 2000.

- Information Technology and the Dual-Degree Program
  Amercian Physical Society, Minneapolis, Minnesota, March 20, 2000.

- Parallel Multiscale Simulations of Nanostructured Materials
  Iowa State University and Ames Research Laboratory, Ames, Iowa, April 3, 2000.

- Multiscale Simulations of Oxidation and Fracture in Nanostructured Solids
  HPaC Seminar, TU Delft, The Netherlands, April 14, 2000.

- Parallel Multiscale Simulations of Nanostructured Materials
  MD Meeting, University of Illinois at Urbana, April 16-17, 2000.

- Massively Parallel Multiscale Simulations of Nanostructured Materials
  Intel Corporation, May 1, 2000.

- Massively Parallel Multiscale Simulations of Nanostructured Ceramics
  American Ceramic Society Symposium on Advances in Theory, Modeling, and Simulations of Materials, St. Louis, Missouri, May 3, 2000.

- Computer Simulations of Ceramic Interfaces
  AFOSR Contractors' Meeting in Ceramic Materials and Composites, St. Louis, Missouri, May 5, 2000.

- Computational Assisted Development of High Temperature Structural Materials
  DoD Challenge User's Group Meeting, Albuquerque, New Mexico, June 8, 2000.

- Parallel Molecular Dynamics Simulations of Nanostructured Materials
  Corsica Meeting on Fracture, June 6-17, 2000.

- Parallel Molecular Dynamics Simulations of Nanostructured Materials
  Canadian Computational Chemistry Meeting, Bishop University, Lennoxville, Quebec, Canada, July 31 - August 3, 2000.

- Simulations of Nanostructured Materials
  TU Delft, The Netherlands, September 25, 2000.

- Multiscale Materials Simulations: Importance of Neutron Scattering
  Argonne National Laboratory, November 20, 2000.

- Multiscale Materials Simulations
  National Research Council, Ottawa, Canada, November 23, 2000.

- Multiscale Simulations of Nanostructured Solids on Massively Parallel Computers
  International Conference on Science & Technology of Nanostructured Materials, Puri, India, January 4-8, 2001.

- Massively Parallel, Multiscale Simulations of Interfacial Materials
  Saclay, France, March 29, 2001.

- Massively Parallel Multiscale Simulations
  DoD Computational Materials Science Workshop, St. Louis, MO, April 24-25, 2001.

- Hybrid Atomistic-Continuum Simulations of Nanopixels
  DoD Users Group Conference, Biloxi, MI, June 18-22, 2001.

- Intercontinental Computational Physics Course
  Niigata University, Japan, June 25, 2001.

- Massively Parallel Simulations of Nanosystems Under Extreme Conditions
  Mission Computing Conference, Washington DC, February 4, 2002.

- Multiscale Simulations of Nanosystems
  IPNS Nanocomposite Workshop, Argonne National Lab, Chicago, IL, March 28, 2002.

- Mulstiscale Simulations of Nanosystems
  Oak Ridge National Lab, TN, April 18, 2002.

- Multiscale Fracture and Nanoindentation Simulations and Visualization
  DoD High-Performance Computing Users Group Conference, Austin, TX, June 12, 2002.

- Mulstiscale Simulation of Atomistic Processes in Nanostructured Materials
  NSF Workshop, University of Illinois at Urbana-Champaign „June 10, 2002.

- Massively Parallel, Multiscale Simulations of Nanostructured Materials
  CIMTEC 2002, Florence, Italy, July 11, 2002.

- Multimillion Atom Simulations of Nanoscale Dynamics and Fracture
  CECAM Workshop, Lyon, France, October 13-15, 2003.

- Multiscale Algorithms and Simulations of Nanosystems
  Joint Physics & Computer Science Colloquium, Florida State University, November 10, 2003.

- Multiscale Algorithms and Simulations of Nnanoceramics and Nanocomposites
  Workshop on Multi-algorithm Methods for Multiscale Simulations (Livermore, Jan. 14-16, 2004).

- Hybrid Multiscale Simulations on Parallel Distributed Computers
  Conference on Dynamics of Disordered Materials on the Nanometer Scale, Hanoi, February 23-27, 2004.

- Multiscale Material Simulation Challenges on a GRID
  APS Meeting, Montreal, March 22-26, 2004.

- Fracture in Glasses and Nanostructured Ceramics: US-European Collaboration
  MRS Meeting, San Francisco, April 15-16, 2004.

- Large-Scale Atomistic Simulations of Nanoindentation and Crack Propagation Under Compression
  DoD-HPCMP 2004 User Group Conference, Williamsburg, VA, June 7-11, 2004.

- *De Novo* Computational Design of Optimum Materials
  Service de Physique et de Chimie des Surfaces et Interfaces, CEA-Saclay, France, July 2, 2004.

- Multiscale Simulations of Nanostructured Ceramics and Glasses
  CMT28, Washington University, St. Louis, September 27 - October 2, 2004.

- Hierarchical Multimillion Atom Simulations of Nanostructured Materials and Nanoscale Devices
  Colloquium in the Department of Materials Science and Engineering, UCLA, October 22, 2004.

- Multimillion Atom Simulations of Structure, Dynamics and Thermo-mechanical Effects
  Army Research Laboratory, Aberdeen Proving Ground, MD, October 29, 2004.

- Hierarchical Atomistic Simulations of Fracture in Nanostructured Materials
  Lorentz Workshop on the Statistical Physics of Pattern Formation and Fracture in Disordered Materials, Leiden, The Netherlands, November 15-19, 2004.

- Hierarchical Multimillion Atom Simulations of Nanostructured Materials and Nanoscale Devices
  TU Delft, The Netherlands, November 19, 2004.

- Large-Scale Atomistic Simulations of Dynamic Fracture in Glasses and Ceramics
  2004 MRS Fall Meeting, Boston, November 29-December 3, 2004.

- Molecular Dynamics Simulations of Structural Phase Transformations in Nanocrystalline Systems
  Caltech Baithak, January 14-15, 2005.

- Multimillion Atom Fracture and Shock Simulations
  45th SANIBEL SYMPOSIUM, St. Simons Island, Georgia, March 5 - 11, 2005.

- Cracks Under Compression
  SVI, Unité Mixte CNRS/Saint-Gobain, France, March 17, 2005.

- Cracks in Brittle Solids
  Department of Chemical Engineering & Materials Science, University of California, Davis, April 25, 2005.

- Molecular Dynamics Simulations of High Strain Rate Deformation and Shock Propagation in Ceramics and Glasses
  DoD-HPCMP 2005 User Group Conference, Nashville, TN, June 27-30, 2005.

- Million-to-Billion Atom Simulation of Chemical and Mechanical Processes
  American Chemical Society Meeting & Exposition, August 28 - September 1, 2005, Washington, DC.

- Wing Crack Dynamics in Silica Glass
  3rd International Workshop on the Flow and Fracture of Advanced Glasses, Pennsylvania State University, October 2–5, 2005.

- Multimillion-atom Simulations of Reactive & Mechanical Behavior of Nano-Engineered Energetic Materials
  Aberdeen, MD, November 16, 2005.

- Hierarchical Million-to-Billion Atom Simulations
  École Polytechnique Montreal, Canada, April 13, 2006.

- Computer "Experiments" on High Strain Rate Deformations in Glasses, Semiconductors, and Ceramics
  Statistical Physics in Mechanics, Grasse - France, June 11-23, 2006

- Multiscale Materials Simulation
  The First US-China Workshop on Neutron Scattering Science and Technology, Beijing China, November 12-15, 2006.

- Multimillion-atom Simulations of Reactive & Mechanical Behavior of Nano-Engineered Energetic Materials,
  Aberdeen, MD, December 11, 2007

- Multimillion-to-Billion Atom Molecular Dynamics Simulations of Deformation, Flow, Fracture & Nanoindentation in Silica Glass
  International Symposium on AMO & HPC: A Seamless Frontier, Kolkatta, India, January 10-12, 2008

- Multimillion-to-Billion Atom Molecular Dynamics Simulations of Deformation, Flow, Fracture & Nanoindentation in Silica Glass
  IUTAM symposium on "Modelling nanomaterials and nanosystems", Aalborg, Denmark, May 19-22, 2008

- Petascale Materials Simulations
  Sixth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), University of British Columbia, Vancouver, BC, Canada, July 19-24, 2008

- Multimillion-to-Billion Atom Molecular Dynamics Simulations of Deformation, Fracture & Nanoindentation in Silica Glass
  TACC 2008, Shanghai, China, September 23-27, 2008

- Keynote Lecture at the SES 2008 meeting on "Multiscale Modeling of Defects in Solids," University of Illinois at Urbana-Champaign, October 12-15 2008

- Petascale Simulations of Hard and Soft Condensed Phase Systems
  Department of Physics, UC Davis, April 30, 2009

- Stress Corrosion Cracking of Silica
  SciDAC Midterm Review, Washington, DC, May 6, 2009

- Deformation, Nanoindentation and Fracture in Silica Glass
  2nd IC4N, Rhodes, Greece, June 29-July 3, 2009

- Deformation, Nanoindentation and Fracture in Silica Glass
  ACSIN 10, Granada, Spain, September 21-25, 2009

- Fracture & Nanoindentation in Silica Glass, and Sulfur Embrittlement of Nickel
  Conference on Multiscale Modeling of Hard & Soft Matter
  Bangalore, India, December 17-20, 2009

- Multimillion-Atom Simulations of Reactive and Mechanical Behavior of Nano-Engineered Energetic Materials
  Annual MURI Review, Aberdeen, MD, March 15, 2010

- Multimillion-Atom Molecular Dynamics Simulations of Poration in Lipid Bilayers
  USC Biomedical Nanoscience Initiative Retreat, November 19, 2010

- Multimillion-Atom Simulations of Bio-Nano Systems
  Physics Colloquium, Arizona State University, Tempe, AZ, October 13, 2011

- Small Interfering RNA Induces Structural Phase Transformation in a Phospholipid Bilayer
  E-MRS, Strasbourg, France, 05/14-18/2012

- Reactive Nanosystems: Multimillion Atom Molecular Dynamics Simulations of Energetic Materials," Joint ONR/AFOSR Advanced Energetic Materials Program Review (August 8, 2012, Arlington, VA)

- Reactive Dissipative Particle Dynamics for Energetic Materials
  ONR meeting, Los Angeles, CA, 02/10-11/2013

- Translocation of Small Interfering RNA and Cholesterol Molecules in Biomembranes
  APS March Meeting, Baltimore, MD, March 18-22, 2013.

- Atomistic simulations of membranes
  2014 DPOLY short course on Multiscale Computational Approaches for Simulating Polymers from Atomistic to Mesoscale, APS March Meeting, Denver, CO, March 3-7, 2014.