Rajiv K. Kalia

ADDRESS: Collaboratory for Advanced Computing and Simulations
University of Southern California, 614 VHE
Los Angeles, CA 90089
Phone: (213) 821-2658; Fax: (213) 821-2664
E-mail: rkalia@usc.edu

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:

2018-Current	Distinguished Affiliate Scientist, DOE Center for Integrated Nanotechnologies, Sandia National Laboratory and Los Alamos National Laboratory.
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) synthesis of layered materials and thermo-mechanical, electrical and optical properties of layered material architectures; 2) self-healing nanoomaterials capable of sensing and repairing damage in harsh chemical environments and in high-temperature/high-pressure operating conditions; 3) structural and dynamic correlation in fluids confined in nanoporous materials; 4) nanoengineered energetic materials and munitions under extreme conditions; 5) shock propagation and pressure-induced structural transformations in nanocluster assemblies and self-assembled monolayers; 6) nucleation and growth of cracks, stress corrosion, and delamination at metal/ceramic, semiconductor/ceramic, and polymer/ceramic interfaces; 7) cholesterol flip-flop dynamics and barriers to small interfering RNA delivery across biomembranes; 8) supercrystals of DNA-functionalized metal nanoparticles; 9) AI driven design, discovery and manufacturing of quantum materials architectures; and 10) AI driven mathematical modeling of viral dynamics in COVID-19 patients.

EDUCATIONAL PROGRAMS

***New Course*:** Developed a course titled **"*Mathematical Methods for Deep Learning*"** for Ph.D. students in the Viterbi School of Engineering.

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

Mathematical methods for deep learning, statistical physics; quantum mechanics; 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). Students and faculty are brought together 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. Follow-on activities 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.

We are also organizing workshops for underrepresented groups of middle school and high school students from inner city schools in Los Angeles. These workshops are also open to adults accompanying student participants. Workshops are held every Saturday from 10 am to noon. Participants are taught Python programming on Raspberry Pi. Our goals are: 1) provide computer

science education to 1500 students in 5 years; and 2) design computational science curricula for middle school and high school students.

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

***Artificial Intelligence Driven Cybermanufacturing of Quantum Material Architectures*:** (Collaborators: Aiichiro Nakano and Han Wang at USC, Radhika Nagpal at Harvard, and Danda Rawat at Howard). Quantum material architectures consist of graphene and other two-dimensional materials, which, when stacked in precise three-dimensional architectures, exhibit unique and tunable mechanical, electrical, optical, and magnetic properties. These three-dimensional architectures have broad potential applications and are highly promising components for microchips, batteries, antennas, chemical and biological sensors, solar-cells and neural interfaces. We are developing a transformative Future Manufacturing platform for quantum material architectures using a cybermanufacturing approach, which combines artificial intelligence, robotics, multiscale modeling, and predictive simulation for the automated and parallel assembly of multiple two-dimensional materials into complex three-dimensional structures. This platform enables future production of high-quality, custom quantum material architectures for broad and critical applications, supporting continued U.S. leadership in technology development. The research advances fundamental knowledge in material physics, nanoscale electronics and photonic science leading the way to manufacturing of future devices, such as twistronics. The research in cybermanufacturing is integrated with innovative educational programs for cross-disciplinary training of scientists and engineers, especially, women and under-represented minorities, in advanced manufacturing, artificial intelligence and quantum structures, as well as engaging the public in future manufacturing concepts.

***Deep Learning for Nanosystems*:** I'm collaborating with scientists at the Center for Integrated Nanotechnologies, Sandia National Laboratory and Los Alamos National Laboratory. We have designed reinforcement learning and unsupervised deep learning models which include various types of Boltzmann machines, dense associative memory neural networks, and autoencoders to analyze and mathematically model material synthesis, electron microscopy/x-ray scattering data and atomistic simulations. We have also developed a function learner neural network to extract physical laws underlying experimental data.

Materials Genome Center: Computational synthesis of materials software project with validation on layered low dimensional functional materials and ultra-fast X-ray laser experiments. (Collaborators: Pulickel M. Ajayan, *Rice University*; Uwe Bergmann and David Fritz, *Linac Coherent Light Source, SLAC*; William A. Goddard, III, *California Institute of Technology*; Kristin A. Persson, *Lawrence Berkeley National Laboratory*; David J. Singh, *University of Missouri*). This project is about layered materials (LMs) genome. We are developing and deliveringing first-principles based computational synthesis software to aid the synthesis of stacked LMs by chemical vapor deposition (CVD), exfoliation and intercalation. The software provides function-property-structure relationships in LMs functionalized by initiated CVD process, is sufficiently general to help synthesis and characterization of other functional nanomaterials. The software suite includes plug-ins for a wide range of properties and processes including band structures and carrier effective masses, oscillator strengths and optical absorption/emission spectra, dielectric function, electric carrier mobility and radiative recombination time, excitonic properties, electrical conductivity, heat and mass transport, and various methods for free energy calculation.

Tracking, Diagnosing and impeding dielectric breakdown using multiscale characterization and simulations **(Multidisciplinary University Research Initiative funded by Office of Naval Research)**. Other team members include Rampi Ramprasad (PI, Director) Georgia Tech, Yang Cao and Greg Sotzing (University of Connecticut), Miko Cakmak (Purdue University), Michael Fayer (Stanford University). The goal of this project is to develop a unified understanding of polymer dielectric degradation and breakdown, in terms of correlations between breakdown behavior and key features of the material, using intricate information meticulously accumulated from the planned experimental and simulation work.

PROPOSALS FUNDED

- R. K. Kalia., A. Nakano, H. Wang (USC); R. Nagpal—PI (Harvard); D. Rawat (Howard University); "*Artificial Intelligence Driven Cybermanufacturing of Quantum Materials Architectures*", NSF, $3,750,000, (September 1, 2020 to August 31, 2025).
- R. K. Kalia, A. Nakano, M. Gupta, O. Prezhdo and P. Vashishta—PI (USC); P. M. Ajayan (Rice); U. Bergmann and D. Fritz (Stanford); W. Goddard (Caltech); K. Persson (UC Berkeley); D. Singh (Missouri); "*Materials Genome Center: Computational Synthesis of Materials Software Project with Validation on Layered Low-Dimensional Functional Materials and Ultra-fast X-ray Laser Experiments*," DOE, DE-SC0014607, $7,500,000, (September 15, 2015 to September 14, 2021).
- R. K. Kalia—PI, P. Vashishta and A. Nakano, "*Self-healing Ceramics and Mechanical Metamaterials*," DOE-BES, DE-FG02-04ER46130, $420,000 (April 15, 2017 to December14, 2020).
- R. K. Kalia, A. Nakano, P. Vashishta—PI, "*Tracking, Diagnosing and Impeding Dielectric Breakdown in Polymers*", ONR, $1,000K (June 1, 2017 to May 31, 2022).
- R. K. Kalia, "*Discovery of New High Frequency Magnetic Materials Enabled by Artificial Intelligence*", Sandia National Laboratory, $180,000 (October 1, 2020 to September 30, 2023).
- R. K. Kalia, "*Beyond Fingerprinting*", Sandia National Laboratory, $285,000 for 3 years (Expected starting date January 1, 2022).
- R. K. Kalia and S. Kumar, "*Data-Driven Modeling of Viral Dynamics in COVID-19 Patients*", Zumberge Research and Innovation Fund, $75,000 (August 1, 2020 to July 31, 2021).

CONFERENCE ACTIVITIES

- Co-Organizer, Focus Sessions on "Emerging Trends in Molecular Dynamics Simulations and Machine Learning", at the 2020 APS March Meeting.
- Co-Organizer, 4 Focus Sessions on "Emerging Trends in Molecular Dynamics Simulations and Data Analytics", at the 2019 APS March Meeting, Boston, MA.
- 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. 14th International Conference on the Physics of Semiconductors, 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 Physics of Intercalation Compounds, 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 Melting, Localization and Chaos, 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 Nonlinear Phenomena at Phase Transitions and Instabilities, 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 6th Pan American Workshop on Condensed Matter Theories, 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 Electron-Hole Droplets in Semiconductors, 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. Recent Progress on Many-Body Theories, 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, Lecture Notes in Physics, 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, Proc. V Int. Symp. on Molten Salts, 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, Condensed Matter Theories, 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
B. P. Feuston, R. K. Kalia, and P. Vashishta, Condensed Matter Theories, vol. **2**, eds. P. Vashishta, R. K. Kalia, and R. F. Bishop, (Plenum, NY), 1987, p. 51.

51. Fragmentation of Silicon Microclusters
B. P. Feuston, R. K. Kalia, and P. Vashishta, Proc. of the Symposium on the Physics and Chemistry of Small Clusters, eds. P. Jena, B. K. Rao, and S. N. Khanna, (Plenum Press, NY), 1987.

52. Molecular Orientational Pinning on a Surface: A Simulated Annealing Study
B. P. Feuston, M. Ma, S. D. Mahanti, and R. K. Kalia, Phys. Rev. **A 37**, 902 (1988).

53. Nature of Gigantic Resistance Fluctuations in Metal-Oxide-Semiconductor Wires
R. K. Kalia, in Condensed Matter Theories, Vol. **3**, eds. J. Arponen, R. F. Bishop, and M. Manninen, (Plenum Press, NY), 1988, p. 197.

54. Ground-State and Finite-Temperature Energetics and Topologies of Germanium Microclusters
G. A. Antonio, B. P. Feuston, R. K. Kalia, and P. Vashishta, J. Chem. Phys. **88**, 7671 (1988).

55. Structural Correlations in Silicon Microclusters
B. P. Feuston, R. K. Kalia, and P. Vashishta, Phys. Rev. **B 37**, 6297 (1988).

56. Variable-Range Hopping Conduction in $Ba_{1-x}K_xBi\ O_{3-y}$ System
B. Dabrowski, D. G. Hinks, J. D. Jorgensen, R. K. Kalia, P. Vashishta, D. R. Richards, D. T. Marx, and A. W. Mitchell, Physica **C 156**, 24 (1988).

57. Structural and Dynamical Correlations in Ag_2Se: A Molecular Dynamics Study of Superionic and Molten Phases
J. P. Rino, Y. M. Hornos, G. A. Antonio, I. Ebbsjö, R. K. Kalia, and P. Vashishta, J. Chem. Phys. **89**, 7542 (1988).

58. Molecular Dynamics Simulation of Mass and Charge Transport in Superionic Conductors, and Structural Correlations in Chalcogenide Glasses
P. Vashishta, J. P. Rino, and R. K. Kalia, Proc. Mat. Sci. Symp., Solid State Ionics, Boston, MA, Nov. 28-Dec. 3, 1988.

59. Rings, Intermediate-Range Order, and Vibrational Spectra of Chalcogenide Glasses
P. Vashishta, R. K. Kalia, and I. Ebbsjö, J. Non-Cryst. Solids **106**, 301 (1988).

60. $SiSe_2$ Glass: A Molecular Dynamics Study
G. A. Antonio, R. K. Kalia, and P. Vashishta, J. Non-Cryst. Solids **106**, 305 (1988).

61. HNC Theory of Medium-Range Order in Glasses
H. Iyetomi, P. Vashishta, and R. K. Kalia, J. Non-Cryst. Solids **106**, 321(1988).

62. Molten Ag_2Se: A Molecular Dynamics Study
Y. M. M. Hornos, G. A. Antonio, J. P. Rino, I. Ebbsjö, R. K. Kalia, and P. Vashishta, Solid State Ionics **32 & 33**, 882 (1989).

63. A Molecular Dynamics Study of Superionic Ag_2Se
J. P. Rino, Y. M. M. Hornos, G. A. Antonio, I. Ebbsjö, R. K. Kalia, and P. Vashishta, Solid State Ionics **32 & 33**, 968 (1989).

64. Atomic Correlations and Intermediate Range Order in Molten and Amorphous $GeSe_2$
P. Vashishta, R. K. Kalia, G. A. Antonio, and I. Ebbsjö, Phys. Rev. Lett. **62**, 1651 (1989).

65. Quantum Molecular Dynamics Study of Electron Transport in an External Field
R. K. Kalia, P. Vashishta, and S. W. de Leeuw, J. Chem. Phys. **90**, 6802 (1989).

66. The Intermediate Range Order in Molten and Glassy $GeSe_2$
H. Iyetomi, P. Vashishta, and R. K. Kalia, Solid State Ionics **32 & 33**, 954 (1989).

67. Structural Correlations and Phonon Density of States in $GeSe_2$ - A Molecular Dynamics Study of Molten and Amorphous States
P. Vashishta, R. K. Kalia, and I Ebbsjö, Phys. Rev. **B 39**, 6034 (1989).

68. Effect of Oxygen Stoichiometry on Superconducting Transition Broadening in $YBa_2Cu_{3\delta}$
D. Shi, M. S. Boley, M. Patel, R. K. Kalia, and P. Vashishta, J. Appl. Phys. **66**, 2074 (1989).

69. Ferroelastic Phase Transition and Phonons in Diatomic Molecular Monolayer
S. Tang, W. Jin, S. D. Mahanti, and R. K. Kalia, Phys. Rev. **B 39,** 677 (1989).

70. Medium-Range Order and Phonon Density of States of a-$GeSe_2$
P. Vashishta and R. K. Kalia, Condensed Matter Theories, vol. 4, ed. J. Keller (Plenum, N.Y., 1989), p. 35.

71. Molecular Dynamics Algorithm on the Connection Machine
D. L. Greenwell, R. K. Kalia, J. C. Patterson, and P. D. Vashishta, in Scientific Applications of the Connection Machine, ed. H. D. Simon, (World Scientific, Singapore), 1989, p. 252; Int. J. High Speed Computing **1**, 321 (1989).

72. Structural Correlations and Vibrational Spectra of Molten and Glassy $GeSe_2$
P. Vashishta, R. K. Kalia, and I. Ebbsjö, Solid State Ionics **32 & 33**, 872 (1989).

73. Integral-Equation Theory of the Origin of Medium-Range Order in Molten and Vitreous Chalcogenides
H. Iyetomi, P. Vashishta, and R. K. Kalia, J. Phys.**:** Condensed Matter. **1**, 2103 (1989).

74. High-Energy Oxygen Phonon Modes and Superconductivity in $Ba_{1-x}K_xBiO_3$--An Inelastic Neutron Scattering Experiment and Molecular Dynamics Simulation
C.-K. Loong, P. Vashishta, R. K. Kalia, M. H. Degani, D. L. Price, J. D. Jorgensen, D. G. Hinks, B. Dabrowski, A. W. Mitchell, D. R. Richards, and Y. Zheng, Phys. Rev. Lett. **62**, 2628 (1989).

75. A Molecular Dynamics Study of $SiSe_2$ Glass
G. A. Antonio, R. K. Kalia, and P. Vashishta, Solid State Ionics **32 & 33**, 950 (1989).

76. Molecular Dynamics Simulations of Classical and Quantum Systems
R. K. Kalia and P. Vashishta, in Proc. Advanced International School on Statistical Physics, eds. S. Prakash and K. N. Pathak, (Wiley Eastern, New Delhi, 1990), p. 142.

77. Electron Bubbles in a Dense Helium Gas
R. K. Kalia and J. Harris, Solid State Commun. **73**, 839 (1990).

78. Interaction Potential for SiO_2 - A Molecular Dynamics Study of Structural Correlations
P. Vashishta, R. K. Kalia, J. P. Rino, and I. Ebbsjö, Phys. Rev. **B 41**, 12197 (1990).

79. Dynamic Simulation of Mixed Quantum-Classical Systems
R. K. Kalia, P. Vashishta, S. W. de Leeuw, and J. Harris, "Strongly Coupled Plasma Physics," ed. S. Ichimaru, (Yamada Science Foundation, Japan), 1990, p. 93.

80. Vibrational Density-of-States, Isotope Effect, and Superconductivity in $Ba_{1-x}K_xBiO_3$
M. H. Degani, R. K. Kalia, and P. Vashishta, "Condensed Matter Theories," ed. V. C. Aguilera-Navarro, (Plenum, New York, 1990), vol. 5, p. 151.

81. Nature of Phonons and Isotope Effect in $Ba_{1-x}K_xBiO_3$
P. Vashishta, M. H. Degani, and R. K. Kalia, "Correlations in Electronic and Atomic Fluids," eds. P. Jena, R. Kalia, P. Vashishta, and M. P. Tosi, (World Scientific, Singapore), 1990, p. 223.

82. Quantum Molecular Dynamics Simulation of Electron Bubbles in a Dense Helium Gas
R. K. Kalia, P. Vashishta, S. W. de Leeuw, and J. Harris, "Condensed Matter Theories", ed. V. C. Aguilera-Navarro, (Plenum, New York, 1990), vol. 5, p. 71.

83. Nature of Phonons, Isotope Effect, and Superconductivity in $Ba_{1-x}K_xBiO_3$
M. H. Degani, R. K. Kalia, and P. Vashishta, "Strongly Coupled Plasma Physics," ed. S. Ichimaru, (Yamada Science Foundation, Japan), 1990, p. 385.

84. Molecular Dynamics Study of the Structure and Dynamics of Network Glasses
P. Vashishta, R. K. Kalia, G. A. Antonio, J. P. Rino, and I. Ebbsjö, Solid State Ionics **40/41**, 175 (1990).

85. Quantum Molecular Dynamics - A New Algorithm for Linear and Non-linear Electron Transport in Disordered Materials
R. K. Kalia, P. Vashishta, L. H. Yang, F. Dech, and J. Rowlan, Int. J. Supercomputer Applications **4**, 22 (1990).

86. Intermediate Range Order in Permanently Densified Vitreous SiO_2 - A Neutron Diffraction and Molecular Dynamics Study
S. Susman, K. J. Volin, D. L. Price, M. Grimsditch, J. P. Rino, R. K. Kalia, P. Vashishta, G. Gwanmesia, Y. Wang, and R. C. Liebermann, Phys. Rev. **B 43**, 1194 (1991).

87. Integral-Equation Approach to Medium Range Order in Molten and Glassy Chalcogenides
H. Iyetomi, P. Vashishta, and R. K. Kalia, Phys. Rev. **B 43**, 1726 (1991).

88. Simulation of Many Electron Correlations in Resonant-Tunneling Diode
A. Nakano, P. Vashishta, and R. K. Kalia, Phys. Rev. **B 43**, 9066 (1991).

89. Electron-Phonon Coupling, Oxygen Isotope Effect, and Superconductivity in $Ba_{1-x}K_xBiO_3$
C. K. Loong, D. G. Hinks, W. Jin, M. H. Degani, D. L. Price, J. D. Jorgensen, B. Dabrowski, A. W. Mitchell, D. R. Richards, Y. Zheng, P. Vashishta, and R. K. Kalia, in Electron-Phonon Interaction in Oxide Superconductors, eds. J. P. Carbotte and R. Baquero, (World Scientific, Singapore, 1991), p. 122.

90. Electron Transport in Disordered Systems - A Nonequilibrium Quantum Molecular Dynamics Approach
A. Nakano, P. Vashishta, and R. K. Kalia, Phys. Rev. **B 43**, 10928 (1991).

91. Oxygen Isotope Effect in Superconducting $Ba_{1-x}K_xBiO_3$ from Phonon Density of States
C. K. Loong, D. G. Hinks, P. Vashishta, W. Jin, R. K Kalia, M. H. Degani, D. L. Price, J. D. Jorgensen, B. Dabrowski, A. W. Mitchell, D. R. Richards, and Y. Zheng, Phys. Rev. Lett. **66**, 3217 (1991).

92. Phonons, Oxygen Isotope Effect and Superconductivity in $Ba_{1-x}K_xBiO_3$
W. Jin, C. K. Loong, D. G. Hinks, P. Vashishta, R. K. Kalia, M. H. Degani, D. L. Price, J. D. Jorgensen, and B. Dabrowski, MRS Symp. Proc. **209**, 895 (1991).

93. Simulation of Correlated Electron Tunneling and Coulomb Blockade in a Quantum-Dot Diode
A. Nakano, R. K. Kalia, and P. Vashishta, Phys. Rev. **B 44**, 8121 (1991).

94. Superconductivity in $Ba_{1-x}K_xBiO_3$ Cubic Oxides
W. Jin, M. H. Degani, R. K. Kalia, P. Vashishta, and C. K. Loong in Condensed Matter Theories, vol. 7, edited by A. N. Proto and J. Aliaga (Plenum, New York, 1992), p. 253.

95. Phonon Density of States and Isotope Effect in $Ba_{1-x}K_xBiO_3$
C. K. Loong, P. Vashishta, R. K. Kalia, W. Jin, M. H. Degani, D. G. Hinks, D. L. Price, J. D. Jorgensen, B. Dabrowski, A. W. Mitchell, D. R. Richards, and Y. Zheng, Phys. Rev. **B 45**, 8052 (1992).

96. Superconductivity in $Ba_{1-x}K_xBiO_3$
W. Jin, M. H. Degani, R. K. Kalia, and P. Vashishta, Phys. Rev. **B 45**, 5535 (1992).

97. Crystalline Fragments in Glasses
G. A. Antonio, R. K. Kalia, A. Nakano, and P. Vashishta, Phys. Rev. **B 45**, 7455 (1992).

98. Probing Localization and Mobility of an Excess Electron in a-Si by Quantum Molecular Dynamics
A. Nakano, P. Vashishta, R. K. Kalia, and L. H. Yang, Phys. Rev. **B 45**, 8363 (1992).

99. Multiple Time-Step Algorithms for Molecular Dynamics Simulations on Intel iPSC/860
A. Nakano, R. K. Kalia, S. de Leeuw, D. L. Greenwell, and P. Vashishta, Proceedings of the Intel Workshop on Technological Focus, Timberline Lodge, OR, April 5-7, 1992.

100. Structure of Rings in Vitreous SiO_2
J. P. Rino, I. Ebbsjö, R. K. Kalia, A. Nakano, and P. Vashishta, Phys. Rev. **B 47**, 3053 (1993).

101. Molecular Dynamics Simulations of Coulombic Systems on Distributed-Memory MIMD Machines
R. K. Kalia, S. W. de Leeuw, A. Nakano, and P. Vashishta, Comput. Phys. Commun. **74**, 316 (1993).

102. Structural and Dynamical Correlations in Glasses
W. Jin, J. P. Rino, P. Vashishta, R. K. Kalia, and A. Nakano in Strongly Coupled Plasma Physics, edited by H. M. Van Horn and S. Ichirmaru, p. 357.

103. Molecular Dynamics Simulation of Network Glasses and Algorithms on Parallel (SIMD and MIMD) Architectures
P. Vashishta, R. K. Kalia, W. Jin, A. Nakano, and D. L. Greenwell in Computer-Aided Innovation of New Materials II, edited by M. Doyama et al. (North Holland, Amsterdam, 1993), p. 235.

104. Dynamical Structure Factor and Vibrational Normal Modes of SiO_2 Glass
W. Jin, R. K. Kalia, and P. Vashishta in Materials Theory and Modeling - MRS Symposium Proceedings, edited by P. D. Bristowe, J. Broughton, and J. M. Newsam (Materials Research Society, Pittsburgh), p. 343.

105. Computer Simulation of Network Glasses and Molecular Dynamics Algorithm on SIMD and MIMD Machines
P. Vashishta, D. L. Greenwell, R. K. Kalia, and A. Nakano in Recent Progress in Many-Body Theories, vol. 3, edited by T. L. Ainworth, C. E. Campbell, and B. E. Krotsceck (Plenum Press, New York, 1992).

106. Quantum Molecular Dynamics Simulation of Electron Transport
A. Nakano, R. K. Kalia, and P. Vashishta in Strongly Coupled Plasma Physics (Univ. of Rochester Press, NY, 1993), p. 465.

107. Structural Transformation, Intermediate-Range Order, and Dynamical Behavior of SiO_2 Glass at High Pressures
W. Jin, R. K. Kalia, P. Vashishta, and J. P. Rino, Phys. Rev. Lett. **71**, 3146 (1993).

108. Resonant Tunneling through a Double Quantum Dot: Phonon-Induced Electron Localization and Effect of a Magnetic Field
A. Nakano, R. K. Kalia, and P. Vashishta, Appl. Phys. Lett. **62**, 3470 (1993).

109. Phonon Dispersion and Density of States of Solid C_{60}
J. Yu, R. K. Kalia, and P. Vashishta, Appl. Phys. Lett. **63**, 3152 (1993).

110. Effect of Pressure on Intermolecular and Intramolecular Phonons in Solid C_{60}
J. Yu, R. K. Kalia, and P. Vashishta, J. Chem. Phys. **99**, 10001 (1993).

111. Parallel Multiple Time-Step Molecular Dynamics with Three-Body Interaction
A. Nakano, R. K. Kalia, and P. Vashishta, Comput. Phys. Commun. **77**, 303 (1993).

112. Atomistic Simulations on Parallel Architectures
R. K. Kalia, W. Jin, S. W. de Leeuw, A. Nakano, and P. Vashishta, Int. J. Quantum Chem. **27**, 781 (1993).

113. Parallel Algorithm for Molecular Dynamics Simulations on Distributed-Memory MIMD Machines
R. K. Kalia, A. Nakano, D. L. Greenwell, P. Vashishta, and S. W. de Leeuw, Supercomputer **54** (X-2), 11 (1993).

114. Structural Correlation of Porous Silica: Molecular Dynamics Simulation on a Parallel Computer
A. Nakano, L. Bi, R. K. Kalia, and P. Vashishta, Phys. Rev. Lett. **71**, 85 (1993).

115. Quantum Dynamical Simulation of Many Electron-Phonon Coupled Systems on Parallel Computers
A. Nakano, R. K. Kalia, and P. Vashishta, Materials Research Society Symposium Proceedings **291**, 73 (1993).

116. Molecular Dynamics Simulation of Aerogel Silica on Parallel Computers
A. Nakano, R. K. Kalia, and P. Vashishta, Materials Research Society Symposium Proceedings **293**, 237 (1993).

117. Parallel Algorithms for Molecular-Dynamics Simulations of Coulombic Systems
W. Li, R. K. Kalia, S. W. de Leeuw, A. Nakano, D. L. Greenwell, and P. Vashishta, Materials Research Society Symposium Proceedings **291**, 267 (1993).

118. Dynamic Structure Factor and Vibrational Properties of SiO_2 Glass
W. Jin, P. Vashishta, R. K. Kalia, and J. P. Rino, Phys. Rev. **B 48**, 9359 (1993).

119. Growth of Pore Interfaces and Roughness of Fracture Surfaces in Porous Silica--Million Particle Molecular-Dynamics Simulations
A. Nakano, R. K. Kalia, and P. Vashishta, Phys. Rev. Lett. **73**, 2336 (1994).

120. Intermolecular and Intramolecular Phonons in Solid C_{60}: Effects of Orientational Disorder and Pressure
J. Yu, L. Bi, R. K. Kalia, and P. Vashishta, Phys. Rev. **B 49**, 5008 (1994).

121. Nonlinear Electron Dynamics in a Resonant Tunneling Diode: Langevin Quantum-Dynamics Simulations on a Massively Parallel Computer
A. Nakano, R. K. Kalia, and P. Vashishta, Appl. Phys. Lett. **64**, 2569 (1994).

122. Molecular-Dynamics Study of Structural Correlation of Porous Silica with use of a Parallel Computer
A. Nakano, L. Bi, R. K. Kalia, and P. Vashishta, Phys. Rev. **B 49**, 9441 (1994).

123. Computer Simulation of Materials Using Parallel Architectures
P. Vashishta, R. K. Kalia, S. W. de Leeuw, D. L. Greenwell, A. Nakano, W. Jin, J. Yu, L. Bi, and W. Li, Comput. Mater. Sci. **2**, 180 (1994).

124. Structural Transformations in Densified Silica Glass: A Molecular Dynamics Simulation Study
W. Jin, R. K. Kalia, P. Vashishta, and J. P. Rino, Phys. Rev. **B 50**, 118 (1994).

125. First Sharp Diffraction Peak and Intermediate-Range Order in Amorphous Silica: Finite-Size Effects in Molecular Dynamics Simulations
A. Nakano, R. K. Kalia, and P. Vashishta, J. Non-Cryst. Sol. **171**, 157 (1994).

126. Multiresolution Molecular Dynamics Algorithm for Realistic Materials Modeling on Parallel Computers
A. Nakano, R. K. Kalia, and P. Vashishta, Comp. Phys. Commun. **83**, 197 (1994).

127. Massively Parallel Algorithms for Computational Nanoelectronics Based on Quantum Molecular Dynamics
A. Nakano, P. Vashishta, and R. K. Kalia, Comp. Phys. Commun. **83**, 181 (1994).

128. Molecular Dynamics and Quantum Molecular Dynamics Simulations on Parallel Architectures
P. Vashishta, R. K. Kalia, A. Nakano, and J. Yu, Int. J. Modern Phys. **C 5**, 281 (1994).

129. Dynamic Correlations in Nanoscale Devices: Quantum Dynamics Simulations on Parallel Architectures
A. Nakano, R. K. Kalia, and P. Vashishta, in High Performance Computing 1994 Grand Challenges in Computer Simulations, ed. A. Tentner (SCS, San Diego, 1994), p. 103.

130. Computer Simulation of Porous Glasses on Parallel Architectures
R. K. Kalia, P. Vashishta, and A. Nakano, in High Performance Computing 1994 Grand Challenges in Computer Simulations, ed. A. Tentner (SCS, San Diego, 1994), p. 158.

131. Effect of Orientational Disorder and Pressure on Phonons in Solid C_{60} - A Tight Binding Molecular Dynamics Study
P. Vashishta, J. Yu, and R. K. Kalia, in High Performance Computing 1994 Grand Challenges in Computer Simulations, ed. A. Tentner (SCS, San Diego, 1994), p. 163.

132. Phonons in Graphitic Tubules - A Tight Binding Molecular Dynamics Study
J. Yu, R. K. Kalia, and P. Vashishta, in High Performance Computing 1994 Grand Challenges in Computer Simulations, ed. A. Tentner (SCS, San Diego, 1994), p. 232.

133. Computational Approach to Nanotechnology on Parallel Architectures
A. Nakano, R. K. Kalia, and P. Vashishta, in High Performance Computing and Its Applications in the Physical Sciences, eds. D. A. Browne et al. (World Scientific, Singapore, 1994), p. 184.

134. Structural and Dynamical Correlations in Stishovite and High Density Silica Glass
W. Jin, R. K. Kalia, and P. Vashishta, in Solid State Ionics - MRS Symposium Proc., eds. G. Nazri, J. M. Tarascon, and M. Armand (Materials Research Society, Pittsburgh) **293**, (1994).

135. Classical and Quantum Simulations on Parallel Computers
P. Vashishta, R. K. Kalia, S. W. de Leeuw, D. L. Greenwell, A. Nakano, W. Jin, J. Yu, L. Bi, and W. Li, in Topics in Condensed Matter Physics, ed. M. P. Das (Nova, 1994), p. 249.

136. Molecular Dynamics and Quantum Molecular Dynamics Simulations on Parallel Architectures
P. Vashishta, R. K. Kalia, A. Nakano, and J. Yu, Proc. 2nd IMACS Conference on Computational Physics, Oct. 6-9, 1993, St. Louis, MO, ed. J. Potvin, (World Scientific, Singapore, 1994), p. 103.

137. Low-Energy Floppy Modes in High-Temperature Ceramics
P. Vashishta, R. K. Kalia, and I. Ebbsjö, Phys. Rev. Lett. **75**, 858 (1995).

138. Dynamics and Morphology of Brittle Cracks: A Molecular-Dynamics Study of Silicon Nitride
A. Nakano, R. K. Kalia, and P. Vashishta, Phys. Rev. Lett. **75**, 3138 (1995).

139. Crystal Structure and Phonon Density of States of High Temperature Ceramic Silicon Nitride
C-K Loong, P. Vashishta, R. K. Kalia, and I. Ebbsjö, Europhysics Lett. **31**, 201 (1995).

140. Molecular-Dynamics Simulations of Covalent Amorphous Insulators on Parallel Computers
P. Vashishta, A. Nakano, R. K. Kalia, and I. Ebbsjö, J. Non-Cryst. Sol. **182**, 59 (1995).

141. Silica Under Very Large Positive and Negative Pressures - Molecular Dynamics Simulations on Parallel Computers
P. Vashishta, R. K. Kalia, A. Nakano, and W. Jin, Int. J. Thermophysics **17**, 169 (1995).

142. Phonons in Graphitic Tubules
J. Yu, R. K. Kalia, and P. Vashishta, Europhysics Lett. **32**, 43 (1995).

143. Phonons in Graphitic Tubules -- A Tight-Binding Molecular Dynamics Study
J. Yu, R. K. Kalia, and P. Vashishta, J. Chem. Phys. **103**, 6697 (1995).

144. Large Scale Molecular-Dynamics Simulations for Porous Silica and Silicon Nitride
R. K. Kalia, A. Omeltchenko, A. Nakano, and P. Vashishta, in High Performance Computer 1995 Grand Challenges in Computer Simulations, ed. A Tentner (SCS, 1995), p. 30.

145. Simulations of Crack Propagation and Fracture in Silica and Silicon Nitride Films on Parallel Computers
P. Vashishta, A. Nakano, and R. K. Kalia, Int. Conf. Solid State Devices and Materials - The Japan Society of Applied Physics, (1995), p. 142.

146. Tight-Binding Molecular Dynamics Study of Graphitic Tubules on Parallel Computers
J. Yu, R. K. Kalia, and P. Vashishta, in High Performance Computing 1995 Grand Challenges in Computer Simulations, ed. A. Tentner (SCS, Phoenix, 1995), p. 147.

147. Molecular Dynamics Simulations of Glasses on Parallel Computers
P. Vashishta, R. K. Kalia, A. Nakano, and I. Ebbsjö, in High Performance Computing 1995 Grand Challenges in Computer Simulations, ed. A. Tentner (SCS, 1995), p. 116.

148. Molecular Dynamics Simulations of Ceramic Films on Parallel Computers
A. Nakano, P. Vashishta, and R. K. Kalia, in High Performance Computing 1995 Grand Challenges in Computer Simulations, ed. A. Tentner (SCS, 1995), p. 189.

149. Million-Particle Simulations of Fracture: Multiresolution Molecular Dynamics Approach on Parallel Architectures
A. Nakano, R. K. Kalia, and P. Vashishta, in Toward Teraflop Computing and New Grand Challenge Applications Conference, eds. R. K. Kalia and P. Vashishta (Nova, 1995), p. 111.

150. Computer Simulation of Materials on Parallel Architectures: Glasses, Solid C_{60}, and Graphitic Tubules
P. Vashishta, R. K. Kalia, W. Jin, J. Yu, and A. Nakano, in Elementary Processes in Dense Plasmas, eds. S. Ichimaru and S. Ogata (Addison-Wesley, Reading, 1995), p. 359.

151. Early Stages of Sintering of Silicon Nitride Nanoclusters: A Molecular Dynamics Study on Parallel Machines
K. Tsuruta, A. Omeltchenko, R. K. Kalia, and P. Vashishta, Europhys. Lett. **33**, 441 (1996).

152. Structure, Mechanical Properties, and Thermal Transport in Microporous Silicon Nitride -- Molecular Dynamics Simulations on a Parallel Machine
A. Omeltchenko, A. Nakano, R. K. Kalia, and P. Vashishta, Europhys. Lett. **33**, 667 (1996).

153. Crack Propagation and Fracture in Ceramic Films -- Million Atom Molecular-Dynamics Simulations on Parallel Computers
P. Vashishta, A. Nakano, R. K. Kalia, and I. Ebbsjö, Mater. Sci. and Eng. **B 37**, 56 (1996).

154. Dynamical Fracture in $SiSe_2$ Nanowires - A Molecular-Dynamics Study
W. Li, R. K. Kalia, and P. Vashishta, Europhys. Lett. **35**, 103 (1996).

155. Dynamics and Morphology of Cracks in Silicon Nitride Films: A Molecular-Dynamics Study on Parallel Computers
A. Nakano, R. K. Kalia, and P. Vashishta, MRS Proc. **408**, 205 (1996).

156. Molecular Dynamics Simulations of $SiSe_2$ Nanowires
W. Li, R. K. Kalia, and P. Vashishta, MRS Proc. **408**, 489 (1996).

157. Distribution of Rings and Intermediate Range Correlations in Silica Glass Under Pressure - A Molecular-Dynamics Study
J. P. Rino, G. Gutiérrez, I. Ebbsjö, R. K. Kalia, and P. Vashishta, MRS Proc. **408**, 333 (1996).

158. Large Scale Molecular Dynamics Study of Amorphous Carbon and Graphite on Parallel Machines
J. Yu, A. Omeltchenko, R. K. Kalia, P. Vashishta, and D. W. Brenner, MRS Proc. **408**, 113. (1996).

159. Early Stages of Sintering of Silicon Nitride Nanoclusters: A Molecular Dynamics Study on Parallel Machines
K. Tsuruta, A. Omeltchenko, R. K. Kalia, and P. Vashishta, MRS Proc. **408**, 181 (1996).

160. Amorphization and Fracture in Silicon Diselenide Nanowires: A Molecular Dynamics Study
W. Li, R. K. Kalia, and P. Vashishta, Phys. Rev. Lett. **77**, 2241 (1996).

161. Sintering of Amorphous Si_3N_4 Nanoclusters: A Molecular-Dynamics Study of Stress Analysis
J. Wang, K. Tsuruta, A. Omeltchenko, R. K. Kalia, and P. Vashishta, MRS Proc. **408**, 573 (1996).

162. Structure, Mechanical Properties, and Thermal Transport in Microporous Silicon Nitride via Parallel Molecular Dynamics
A. Omeltchenko, A. Nakano, R. K. Kalia, and P. Vashishta, MRS Proc. **408**, 175 (1996).

163. Fracture, Sintering, and Thermal Transport in Silicon Nitride by Parallel Molecular Dynamics Simulations
R. K. Kalia, A. Nakano, A. Omeltchenko, K. Tsuruta, P. Vashishta, and J. Wang, Proc. Condensed Matter Theory Workshop in Venezuela, (Nova, N.Y., 1996).

164. Large-Scale Simulations of Amorphous Materials
P. Vashishta, A. Nakano. R. K. Kalia, and I. Ebbsjö, Proc. Condensed Matter Theory Workshop in Venezuela, (Nova, N.Y., 1996).

165. Million Atom Molecular Dynamics Simulations of Materials on Parallel Computers
P. Vashishta, R. K. Kalia, W. Li, A. Nakano, A. Omeltchenko, K. Tsuruta, J. Wang, and I. Ebbsjö, "Current Opinion in Solid State & Material Science," vol. 1/6, edited by A. M. Stoneham and M. L. Klein.

166. Million Atom Molecular Dynamics Simulation of Nanophase Silicon Nitride
R. K. Kalia, A. Nakano, A. Omeltchenko, K. Tsuruta, and P. Vashishta, in Chemistry and Physics of Nanostructures, eds. E. Ma et al., (TMS, Warrendale, PA), 1997, p. 89.

167. Morphology of Pores and Interfaces and Mechanical Behavior of Nanocluster-Assembled Silicon Nitride Ceramic
R. K. Kalia, A. Nakano, K. Tsuruta, and P. Vashishta, Phys. Rev. Lett. **78**, 689 (1997).

168. Role of Ultrafine Microstructures in Dynamic Fracture in Nanophase Silicon Nitride
R. K. Kalia, A. Nakano, A. Omeltchenko, K. Tsuruta, and P. Vashishta, Phys. Rev. Lett. **78**, 2144 (1997).

169. Crack Propagation and Fracture in a Graphite Sheet: A Molecular-Dynamics Study on Parallel Computers
A. Omeltchenko, J. Yu, R. K. Kalia, and P. Vashishta, Phys. Rev. Lett. **78**, 2148 (1997).

170. Direct Atomistic Simulation of Quartz Crystal Oscillators. I. Bulk Properties
J. Q. Broughton, C. A. Meli, P. Vashishta, and R. K. Kalia, Phys. Rev. **B 56**, 611 (1997).

171. Dynamics of Consolidation and Crack Growth in Nanocluster-Assembled Amorphous Silicon Nitride
K. Tsuruta, A. Nakano, R. K. Kalia, and P. Vashishta, J. Am. Ceram. Soc. **81**, 433 (1998).

172. Multimillion-Atom Molecular Dynamics Simulation of Atomic Level Stresses in $Si(111)/Si_3N_4(0001)$ Nanopixels
M. E. Bachlechner, A. Omeltchenko, A. Nakano, R. K. Kalia, P. Vashishta, I. Ebbsjö, A. Madhukar, and P. Messina, Appl. Phys. Lett. **72**, 1969 (1998).

173. Multilevel Algorithms for Large-scope Molecular Dynamics Simulations of Nanostructures on Parallel Computers
A. Nakano, R. K. Kalia, and P. Vashishta, VLSI Design **8**, 123 (1998).

174. Atomistic Simulation of Nanostructured Materials Using Parallel Multiresolution Algorithms
A. Nakano, M. E. Bachlechner, T. J. Campbell, R. K. Kalia, A. Omeltchenko, K. Tsuruta, P. Vashishta, S. Ogata, I. Ebbsjö, and A. Madhukar, IEEE Comput. Sci. & Eng. **5** (4), 68 (1998).

175. Multimillion Atom Molecular Dynamics Simulations of Ceramic Materials and Interfaces on Parallel Computers
P. Vashishta, M. E. Bachlechner, R. K. Kalia, A. Nakano, A. Omeltchenko, K. Tsuruta, I. Ebbsjö, and A. Madhukar, in Proc. Special Symposium on Advanced Materials, eds. T. Imura, H. Fujita, T. Ichinokawa, and H. Kawazoe (Nagoya, Japan, 1998), p. 47.

176. Oxidation Dynamics of Nanophase Aluminum Clusters: A Molecular Dynamics Study
S. Ogata, T. J. Campbell, K. Tsuruta, A. Nakano, R. K. Kalia, P. Vashishta, and C.-K. Loong, Materials Research Society Symposium Proceedings **481**, 625 (1998).

177. Structural Correlations and Stress Distribution at Silicon/Silicon Nitride Interface
M. E. Bachlechner, A. Omeltchenko, K. Tsuruta, A. Nakano, R. K. Kalia, P. Vashishta, and A. Madhukar, in Computer-Aided Design of High-Temperature Materials, eds. A. Pechenik, R. K. Kalia, and P. Vashishta (Oxford Univ. Press, 1999), p. 244.

178. Multilevel Algorithms for Computational High-Temperature Materials Research
A. Nakano, T. Campbell, R. K. Kalia, and P. Vashishta, in Computer-Aided Design of High-Temperature Materials, eds. A. Pechenik, R. K. Kalia, and P. Vashishta (Oxford Univ. Press, 1999), p. 422.

179. Dynamic Fracture in Nanophase Ceramics and Diamond Films: Multimillion Atom Parallel Molecular-Dynamics Simulations
A. Omeltchenko, K. Tsuruta, A. Nakano, R. K. Kalia, and P. Vashishta, in Computer-Aided Design of High-Temperature Materials, eds. A. Pechenik, R. K. Kalia, and P. Vashishta (Oxford Univ. Press, 1999), p. 81.

180. Structure and Dynamics of Consolidation and Fracture of Nanophase Ceramics via Parallel Molecular Dynamics
K. Tsuruta, J. Wang, A. Nakano, A. Omeltchenko, R. K. Kalia, and P. Vashishta, in Computer-Aided Design of High-Temperature Materials, eds. A. Pechenik, R. K. Kalia, and P. Vashishta (Oxford Univ. Press, 1999), p. 323.

181. Structural Correlations in Amorphous SiO_2 at High Pressures
J. P. Rino, A. Nakano, R. K. Kalia, and P. Vashishta, in Computer-Aided Design of High-Temperature Materials, edited by A. Pechenik, R. K. Kalia, and P. Vashishta (Oxford Univ. Press, Oxford, 1999), p. 374.

182. Parallel Molecular Dynamics Simulations of High Temperature Ceramics
A. Chatterjee, T. Campbell, R. K. Kalia, A. Nakano, A. Omeltchenko, K. Tsuruta, P. Vashishta, Journal of the European Ceramic Society **19**, 2257 (1999).

183. Structural Correlations at Si/Si_3N_4 Interface and Atomic Stress in Si/Si_3N_4 Nanopixels--10 Million-atom Molecular Dynamics Simulation on Parallel Computers
M. E. Bachlechner, R. K. Kalia, A. Nakano, A. Omeltchenko, P. Vashishta, I. Ebbsjö, A. Madhukar, and G.-L. Zhao, Journal of the European Ceramic Society **19**, 2265 (1999).

184. Structural Correlations and Mechanical Behavior in Nanophase Silica Glasses
T. Campbell, R. K. Kalia, A. Nakano, F. Shimojo, K. Tsuruta, and P. Vashishta, Phys. Rev. Lett. **82**, 4018 (1999).

185. Dynamics of Oxidation of Aluminum Nanoclusters Using Variable Charge Molecular-Dynamics Simulations on Parallel Computers
T. Campbell, R. K. Kalia, A. Nakano, P. Vashishta, S. Ogata, and S. Rodgers, Phys. Rev. Lett. **82**, 4866 (1999).

186. Pressure Induced Structural Transformation in Nanocluster Assembled Gallium Arsenide
S. Kodiyalam, A. Chatterjee, I. Ebbsjö, R. K. Kalia, H. Kikuchi, A. Nakano, J. P. Rino,and P. Vashishta, Materials Research Society Symposium Proceedings **536**, 545 (1999).

187. Molecular Dynamics Simulations of Nanoindentation of Silicon Nitride
P. Walsh, A. Omeltchenko, H. Kikuchi, R. K. Kalia, A. Nakano, and P. Vashishta, Materials Research Society Symposium Proceedings **539**, 119 (1999).

188. Multimillion Atom Molecular Dynamics Simulations of Glasses and Ceramic Materials
P. Vashishta, R. K. Kalia, and A. Nakano, in *Physics of Glasses: Structure and Dynamics*, eds. P. Jund and R. Jullien (American Institute of Physics, Melville, NY, 1999), p. 149.

189. Scalable Molecular Dynamics, Visualization, and Data Management Algorithms for Materials Simulations
A. Nakano, R. K. Kalia, and P. Vashishta, Computing in Science & Engineering **1** (5), 39 (1999).

190. Large-scale Atomistic Simulation of Dynamic Fracture
P. Vashishta, R. K. Kalia, and A. Nakano, Computing in Science & Engineering **1** (5), 56 (1999).

191. Variable-charge Interatomic Potentials for Molecular Dynamics Simulations of TiO_2
S. Ogata, H. Iyetomi, K. Tsuruta, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta Journal of Applied Physics **86**, 3036 (1999).

192. Incipient Phase Separation in Ag/Ge/Se Glasses: Clustering of Ag Atoms
H. Iyetomi, P. Vashishta, and R. K. Kalia, J. Non-Crystalline Solids **262**, 135 (2000).

193. Stress Domains in Si(111)/Si_3N_4(0001) Nanopixel – 10 Million-atom Molecular Dynamics Simulations on Parallel Computers
A. Omeltchenko, M. E. Bachlechner, A. Nakano, R. K. Kalia, P. Vashishta, I. Ebbsjö, A. Madhukar, and P. Messina, Phys. Rev. Lett. **84**, 318 (2000).

194. Atomistic Simulations of Nanostructures
A. Nakano, R. K. Kalia, and P. Vashishta, Solid State Physics (Tokyo) **35**, 1 (2000).

195. Dislocation Emission at Silicon/Silicon Nitride Interface - A Million Atom Molecular Dynamics Simulation on Parallel Computers
M. E. Bachlechner, A. Omeltchenko, A. Nakano, R. K. Kalia, P. Vashishta, I. Ebbsjö, and A. Madhukar, Phys. Rev. Lett. **84**, 322 (2000).

196. Molecular Dynamics Simulation of Pressure Induced Structural Transformation in Silicon Carbide
F. Shimojo, I. Ebbsjö, R. K. Kalia, A. Nakano, J. P. Rino, and P. Vashishta, Phys. Rev. Lett. **84**, 3338 (2000).

197. Topology of Amorphous Gallium Arsenide on Intermediate Length Scales: A Molecular Dynamics Study
I. Ebbsjö, R. K. Kalia, A. Nakano, J. P. Rino, and P. Vashishta, Journal of Applied Physics **87**, 7708 (2000).

198. Amorphization and Anisotropic Fracture Dynamics during Nanoindentation of Silicon Nitride - A Multi-million Atom Molecular Dynamics Study
P. Walsh, R. K. Kalia, A. Nakano, P. Vashishta, and S. Saini, Applied Physics Letters **77**, 4332 (2000).

199. Sintering, Structure, and Mechanical Properties of Nanophase SiC: A Molecular Dynamics and Neutron Scattering Study
A. Chatterjee, R. K. Kalia, C.-K. Loong, A. Nakano, A. Omeltchenko, K. Tsuruta, P. Vashishta, M. Winterer, and S. Klein, Applied Physics Letters **77**, 1132 (2000).

200. Scalable I/O of Large-scale Molecular Dynamics Simulations: A Data Compression Algorithm
A. Omeltchenko, T. J. Campbell, R. K. Kalia, X. Liu, A. Nakano, and P. Vashishta, Computer Physics Communications **131**, 78 (2000).

201. Multiresolution Algorithms for Massively Parallel Molecular Dynamics Simulations of Nanostructured Materials
R. K. Kalia, T. J. Campbell, A. Chatterjee, A. Nakano, P. Vashishta, and S. Ogata Computer Physics Communications **128**, 245 (2000).

202. Multimillion Atom Simulations of Nanostructured Materials on Parallel Computers - Sintering and Consolidation, Fracture, and Oxidation
P. Vashishta, M. E. Bachlechner, T. J. Campbell, R. K. Kalia, H. Kikuchi, S. Kodiyalam, A. Nakano, S. Ogata, F. Shimojo, and P. Walsh, Supplement of Progress of Theoretical Physics **138**, 175 (2000).

203. Intercluster Interaction of TiO_2 Nanoclusters using Variable-charge Interatomic Potentials
S. Ogata, H. Iyetomi, K. Tsuruta, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta Materials Research Society Symposium Proceedings **581**, 667 (2000).

204. Large-scale Atomistic Modeling of Nanoelectronic Structures
A. Nakano, M. E. Bachlechner, P. Branicio, T. J. Campbell, I. Ebbsjö, R. K. Kalia, A. Madhukar, S. Ogata, A. Omeltchenko, J. P. Rino, F. Shimojo, P. Walsh, and P. Vashishta IEEE Transactions on Electron Devices **47**, 1804 (2000).

205. A Scalable Molecular Dynamics Algorithm Suite for Materials Simulations: Design-space Diagram on 1,024 Cray T3E Processors
F. Shimojo, T. J. Campbell, R. K. Kalia, A. Nakano, P. Vashishta, S. Ogata, and K. Tsuruta, Future Generation Computer Systems **17**, 279 (2000).

206. Role of Atomic Charge Transfer on Sintering of TiO_2 Nanoparticles: Variable-charge Molecular Dynamics
S. Ogata, H. Iyetomi, K. Tsuruta, F. Shimojo, A. Nakano, R. K. Kalia, and P. Vashishta, Journal of Applied Physics **88**, 6011-6015 (2000).

207. Multi-million Atom Molecular Dynamics Simulations of Stresses in Si(111)/a-Si_3N_4 Nanopixels
M. E. Bachlechner, A. Omeltchenko, P. Walsh, A. Nakano, R. K. Kalia, P. Vashishta, I. Ebbsjö, and A. Madhukar, Materials Research Society Symposium Proceedings **592**, 369 (2000).

208. Multimillion-atom Simulations of Atomic-level Surface Stresses and Migration Processes on InAs/GaAs Mesas
X. Su, R. K. Kalia, A. Madhukar, A. Nakano, and P. Vashishta, Materials Research Society Symposium Proceedings **584**, 269 (2000).

209. Recent Progress in Nanomaterials Simulations
H. Iyetomi, S. Ogata, H. Kikuchi, F. Shimojo, K. Tsuruta, A. Nakano, R. K. Kalia, and P. Vashishta, Material Integration (Kyoto), **14** (1), 3-8 (2001).

210. Multiscale Simulation of Materials
A. Nakano, M. E. Bachlechner, R. K. Kalia, E. Lidorikis, P. Vashishta, G. Z. Voyiadjis, T. J. Campbell, S. Ogata, and F. Shimojo, Computing in Science & Engineering **3**, 56-66 (2001).

211. Grain Boundaries in Gallium Arsenide Nanocrystals under Pressure: A Parallel Molecular-Dynamics Study
S. Kodiyalam, R. K. Kalia, H. Kikuchi, A. Nakano, F. Shimojo and P. Vashishta, Phys. Rev. Lett. **86**, 55-58 (2001).

212. Coupling Length Scales for Multiscale Atomistic-Continuum Simulations: Atomistically-Induced Stress Distributions in Si/Si_3N_4 Nanopixels
E. Lidorikis, M. E. Bachlechner, R. K. Kalia, A. Nakano, P. Vashishta, and G. Z. Voyiadjis, Phys. Rev. Lett. **87**, 086104 (2001).

213. Million-atom Molecular Dynamics Simulation of Flat InAs Overlayers with Self-limiting Thickness on GaAs Nanomesas
X. Su, R. K. Kalia, A. Madhukar, A. Nakano, and P. Vashishta, Applied Physics Letters, **78**, 3717 (2001).

214. Large-scale Molecular Dynamics Simulations of Materials on Parallel Computers
A. Nakano, T. J. Campbell, R. K. Kalia, S. Kodiyalam, S. Ogata, F. Shimojo, P. Vashishta, and P. Walsh in *Advanced Computing and Analysis*, edited by P. Bhat and M. Kaseman (American Institute of Physics, Melville, NY, 2001), pp. 57-62.

215. Coupling of Length Scales: Hybrid Molecular Dynamics and Finite Element Approach for Multiscale Nanodevice Simulations
E. Lidorikis, M. E. Bachlechner, R. K. Kalia, G. Z. Voyiadjis, A. Nakano, and P. Vashishta, MRS Symposium Proceedings **653**, Z9.3.1 - Z9.3.6, (2001).

216. Linear-scaling Density Functional Theory Calculations of Electronic Structure Based on Real-space Grids: Design, Analysis, and Scalability Test of Parallel Algorithms
F. Shimojo, R. K. Kalia. A. Nakano, and P. Vashishta, Computer Physics Communications **140**, 303-314 (2001).

217. Structural Transformation, Amorphization, and Fracture in Nanowires: A Multi-million Atom Molecular Dynamics Study
P. Walsh, W. Li, R. K. Kalia, A. Nakano, P. Vashishta, and S. Saini, Applied Physics Letters **78**, 3328-3330 (2001).

218. Hybrid Finite-element/Molecular-dynamics/Electronic-density-functional Approach to Materials Simulations on Parallel Computers
S. Ogata, E. Lidorikis, F. Shimojo, A. Nakano, P. Vashishta, and R. K. Kalia, Computer Physics Communications **138**, 143-154 (2001).

219. Scalable Atomistic Simulation Algorithms for Materials Research
A. Nakano, R. K. Kalia, P. Vashishta, T. J. Campbell, S. Ogata, F. Shimojo, S. Saini, in *Proceedings of Supercomputing 2001* (IEEE/ACM, New York, NY, 2001).

220. Multimillion Atom Simulation of Materials on Parallel Computers—Nanopixel, Interfacial Fracture, Nanoindentation, and Oxidation
P. Vashishta, M. E. Bachlechner, A. Nakano, T. J. Campbell, R. K. Kalia, S. Kodiyalam, S. Ogata, F. Shimojo, and P. Walsh, Applied Surface Science **182**, 258-264 (2001).

221. Critical Lateral Size for Domain Formation in InAs/GaAs Square Nanomesas: A Multi-million-atom Molecular Dynamics Study
X. Su, R. K. Kalia, A. Madhukar, A. Nakano, and P. Vashishta , Applied Physics Letters **79**, 4577-4579 (2001).

222. Initial Stages of Sintering of TiO_2 Nanoparticles: Variable-charge Molecular Dynamics Simulations
S. Ogata, H. Iyetomi, K. Tsuruta, F. Shimojo, A. Nakano, P. Vashishta, R. K. Kalia, and C.-K. Loong, Materials Research Society Symposium Proceedings **634**, B.7.6.1-B.7.6.6 (2001).

223. Hybrid Electronic-Density-Functional/Molecular-Dynamics Simulation on Parallel Computers: Oxidation of Si Surface
S. Ogata, F. Shimojo, A. Nakano, R. K. Kalia, and P. Vashishta, Materials Research Society Symposium Proceedings **653**, Z.6.5.1-Z.6.5.6 (2001).

224. Atomistic Simulations of Nanoceramics
C. L. Rountree, L. Van Brutzel, E. Lidorikis, A. Nakano, R. K. Kalia, and P. Vashishta, in *Proceedings of CINTEC 2002, 10th International Ceramic Congress and 3rd Forum on New Materials*, edited by P. Vincenzini (Florence, Italy, July 14-18, 2002).

225. Collaborative Simulation Grid: Multiscale Quantum-Mechanical/Classical Atomistic Simulations on Distributed PC Clusters in the US and Japan
H. Kikuchi, R. K. Kalia, A. Nakano, P. Vashishta, H. Iyetomi, S. Ogata, T. Kouno, F. Shimojo, K. Tsuruta, and S. Saini, in *Proceedings of Supercomputing 2002* (ACM, New York, NY, 2002).

226. Dynamic Fracture Mechanisms in Nanostructured and Amorphous Silica Glasses: Million-Atom Molecular Dynamics Simulations
L. Van Brutzel, C. L. Rountree, R. K. Kalia, A. Nakano, and P. Vashishta, Materials Research Society Symposium Proceedings 703, V.3.9.1-V.3.9.6 (2002).

227. Improving Interactivity of a Parallel and Distributed Immersive Walkthrough Application for Very Large Datasets with Artificial Neural-Network-Based Machine Learning
X. Liu, A. Sharma, P. Miller, W. Zhao, A. Nakano, R. K. Kalia, and P. Vashishta, in *Proceedings of the International Conference on Parallel and Distributed Processing Techniques and Applications, Vol. IV* (CSREA Press, Las Vegas, NV, 2002) pp. 2054-2058.

228. Info-bio-nano Interface: High-Performance Computing and Visualization
P. Vashishta, R. K. Kalia, and A. Nakano, in *Proceedings of High Performance Computing - HiPC 2002*, edited by S. Sahni, V. K. Prasanna, and U. Shukla (Springer, Berlin, 2002) pp. 3-8.

229. Multimillion Atom Simulations of Nanosystems on Parallel Computers
P. Vashishta, R. K. Kalia, S. Kodiyalam, E. Lidorikis, A. Nakano, P. Walsh, M. E. Bachlechner, T. J. Campbell, S. Ogata, and F. Shimojo, in *Proceedings of the International Symposium on Computational Science and Engineering 2002*, edited by A. Ukawa (Japan Society for the Promotion of Science, Tokyo, Japan, 2002).

230. Pressure induced Structural Transformation in Gallium Arsenide: A Molecular-Dynamics Study
J. P. Rino, A. Chatterjee, I. Ebbsjö, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta, Phys. Rev. **B 65**, 195206:1-5 (2002).

231. Scalable Atomistic Simulation Algorithms for Materials Research
A. Nakano, R. K. Kalia, P. Vashishta, T. J. Campbell, S. Ogata, F. Shimojo, and S. Saini Scientific Programming **10**, 263-270 (2002).

232. Atomistic Aspects of Crack Propagation in Brittle Materials: Multimillion Atom Molecular Dynamics Simulations
C. L. Rountree, R. K. Kalia, E. Lidorikis, A. Nakano, L. Van Brutzel, and P. Vashishta, Annual Review of Materials Research **32**, 377-400 (2002).

233. Scalability of a Low-cost Multi-Teraflop Linux Cluster for High-end Classical Atomistic and Quantum Mechanical Simulations
H. Kikuchi, R. K. Kalia, A. Nakano, P. Vashishta, F. Shimojo, and S. Saini, in *Proceedings of the International Parallel and Distributed Processing Symposium* (IEEE/ACM, Nice, France, 2003).

234. Large-scale Atomistic Simulation of Nanostructured Materials on Parallel Computers
P. Vashishta, M. E. Bachlechner, T. J. Campbell, R. K. Kalia, H. Kikuchi, S. Kodiyalam, A. Nakano, S. Ogata, F. Shimojo, and P. Walsh, in *Phase Transformations and Evolution in Materials*, edited by P. E. A. Turchi and T. Gonis (The Minerals, Metals & Materials Society, Warrendale, PA).

235. Hybrid Quantum Mechanical/Molecular Dynamics Simulation on Parallel Computers: Density Functional Theory on Real-space Multigrids
S. Ogata, F. Shimojo, A. Nakano, P. Vashishta, and R. K. Kalia, Computer Physics Communications **149**, 30-38 (2002).

236. Multiresolution Atomistic Simulations of Dynamic Fracture in Nanostructured Ceramics and Glasses
R. K. Kalia, A. Nakano, P. Vashishta, C. L. Rountree, L. Van Brutzel, and S. Ogata, International Journal of Fracture **121**, 71-79 (2003).

237. Nanoindentation of Silicon Nitride: A Multi-million Atom Molecular Dynamics Study
P. Walsh, A. Omeltchenko, R. K. Kalia, A. Nakano, P. Vashishta, and S. Saini, Applied Physics Letters **82**, 118-120 (2003).

238. Structural, Mechanical, and Vibrational Properties of $Ga_{1-x}In_xAs$ Alloy: A Molecular Dynamics Study
P. S. Branicio, R. K. Kalia, A. Nakano, J. P. Rino, F. Shimojo, and P. Vashishta, Applied Physics Letters **82**, 1057-1059 (2003).

239. Large Multidimensional Data Visualization for Materials Science
A. Sharma, R. K. Kalia, A. Nakano, and P. Vashishta
IEEE Computing in Science and Engineering **5** (2), 26-33 (2003).

240. Multimillion Atom Molecular Dynamics Simulations of Nanoparticles on Parallel Computers
P. Vashishta, R. K. Kalia, and A. Nakano, Journal of Nanoparticle Research **5**, 119-135 (2003).

241. Molecular Dynamics Study of Structural, Mechanical, and Vibrational Properties of Crystalline and Amorphous $Ga_{1-x}In_xAs$ alloy:
P. S. Branicio, J. P. Rino, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Applied Physics **94**, 3840-3848 (2003).

242. Immersive and Interactive Exploration of Billion-Atom Systems
A. Sharma, P. Miller, X. Liu, A. Nakano, R. K. Kalia, P. Vashishta, W. Zhao, T. J. Campbell, and A. Haas, Presence: Teleoperators and Virtual Environments **12**, 85-95 (2003).

243. Scalable and Portable Implementation of the Fast Multipole Method on Parallel Computers
S. Ogata, T. J. Campbell, R. K. Kalia, A. Nakano, P. Vashishta, and S. Vemparala, Computer Physics Communications **153**, 445-461 (2003).

244. Multimillion Atom Molecular Dynamics Simulations of Nanoparticles on Parallel Computers
P. Vashishta, R. K. Kalia, and A. Nakano, Journal of Nanoparticle Research **5**, 119-135 (2003).

245. InAs/GaAs Square Nanomesas: Multimillion-atom Molecular Dynamics Simulations on Parallel Computers
X. Su, R. K. Kalia, A. Nakano, P. Vashishta, and A. Madhukar, Journal of Applied Physics **94**, 6762-6773 (2003).

246. Scalable Multiresolution Algorithms for Classical and Quantum Molecular Dynamics with Applications to Nanosystems
A. Nakano, T. J. Campbell, R. K. Kalia, S. Kodiyalam, S. Ogata, F. Shimojo, X. Su, and P. Vashishta, in *Handbook of Numerical Analysis, Volume X, Computational Chemistry*, edited by C. Le Bris (Elsevier, Amsterdam, The Netherlands, 2003), pp. 639-666.

247. Mechanisms of Stress Corrosion Cracking in Si: A Hybrid Quantum-Mechanical/Molecular-Dynamics Simulation
R. Belkada, S. Ogata, F. Shimojo, A. Nakano, P. Vashishta, and R. K. Kalia, Materials Research Society Symposium Proceedings **750**, 531-536 (2003).

248. High-end Classical/Quantum Atomistic Simulations of Fracture
R. K. Kalia, A. Nakano, P. Vashishta, and C. L. Rountree in *Proceedings of the 2003 Users Group Conference* (IEEE Computer Society, Los Alamitos, CA, 2003) pp. 36-39.

249. Multiple Grains in Nanocrystals: Effect of Initial Shape and Size on Transformed Structures Under Pressure
S. Kodiyalam, R. K. Kalia, A. Nakano, and P. Vashishta, Phys. Rev. Lett. **93**, 203401:1-4 (2004).

250. Atomistic Mechanisms for Wurtzite-to-Rocksalt Structural Transformation in Cadmium Selenide Under Pressure
F. Shimojo, S. Kodiyalam, I. Ebbsjö, R. K. Kalia, A. Nakano, and P. Vashishta, Physical Review B **70**, 184111: 1-6 (2004).

251. Environmental Effects of H_2O on Fracture Initiation in Silicon: A Hybrid Electronic-Density-Functional/Molecular-Dynamics Study
S. Ogata, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Applied Physics **95**, 5316-5323 (2004).

252. Nanoindentation-Induced Amorphization in Silicon Carbide
I. Szlufarska, R. K. Kalia, A. Nakano, and P. Vashishta, Applied Physics Letters **85**, 378-380 (2004).

253. Short- and Intermediate-Range Structural Correlations in Amorphous Silicon Carbide (a-SiC): A Molecular Dynamics Study
J. P. Rino, I. Ebbsjö, P. S. Branicio, R. K. Kalia, A. Nakano, and P. Vashishta, Physical Review B **70**, 045207: 1-11 (2004).

254. Large-Scale Molecular Dynamics Simulations of Alkanethiol Self-Assembled Monolayers
S. Vemparala, B. B. Karki, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Chemical Physics **121**, 4323-4330 (2004).

255. Electric Field Induced Switching of Poly (ethylene glycol) (PEG) Terminated Self-Assembled Monolayers: A Parallel Molecular Dynamics Simulation
S. Vemparala, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Chemical Physics **121**, 5427-5433 (2004).

256. Scalable and Portable Visualization of Large Atomistic Datasets
A. Sharma, R. K. Kalia, A. Nakano, and P. Vashishta, Computer Physics Communications **163**, 53-64 (2004).

257. Dynamics of wing cracks and nanoscale damage in glass
Z. Lu, K. Nomura, A. Sharma, W. Wang, C. Zhang, A. Nakano, R. K. Kalia, P. Vashishta, E. Bouchaud, and C. L. Rountree, Phys. Rev. Lett. **95**, 135501: 1-4 (2005).

258. Atomistic Mechanisms of Amorphization During Nanoindentation of SiC: A Molecular Dynamics Study
I. Szlufarska, R. K. Kalia, A. Nakano, and P. Vashishta, Phys. Rev. B **71**, 174113:1-11 (2005).

259. Atomistic processes during nanoindentation of amorphous silicon carbide
I. Szlufarska, R. K. Kalia, A. Nakano, and P. Vashishta, Applied Physics Letters **86**, 021915: 1-3 (2005).

260. Molecular dynamics simulations of the nano-scale room-temperature oxidation of aluminum single crystals
A. Hasnaoui, O. Politano, J. M. Salazar, G. Aral, R. K. Kalia, A. Nakano, and P. Vashishta, Surface Science **579**, 47-57 (2005).

261. Oxidation of Aluminum Nanoclusters
T. J. Campbell, G. Aral, S. Ogata, R. K. Kalia, A. Nakano, and P. Vashishta, Phys. Rev. B **71**, 205413:1-14 (2005).

262. Coupling atomistic and continuum length scales in heteroepitaxial systems: Multiscale molecular-dynamics/finite-element simulations of strain relaxation in Si/Si_3N_4 nanopixels
E. Lidorikis, M. E. Bachlechner, R. K. Kalia, A. Nakano, and P. Vashishta, Phys. Rev. B **72**, 115338: 1-16 (2005).

263. Brittle dynamic fracture of crystalline 3C-SiC via molecular dynamics simulation
H. Kikuchi, A. Nakano, R. K. Kalia, P. Vashishta, P. S. Branicio, and F. Shimojo, Journal of Applied Physics **98**, 103524 (2005).

264. Effect of geometry on the stress relaxation in InAs/GaAs rectangular nano-mesas: Multimillion-atom molecular dynamics simulations
M. A. Makeev, R. K. Kalia, A. Nakano, P. Vashishta, and A. Madhukar, Journal of Applied Physics **98**, 114313: 1-8 (2005).

265. Embedded divide-and-conquer algorithm on hierarchical real-space grids: Parallel molecular dynamics simulation based on linear-scaling density functional theory
F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta, Computer Physics Communications **167**, 151-164 (2005).

266. Strategic application of Asia-Pacific GRID for ultrascale materials simulations
A. Nakano, R. K. Kalia, P. Vashishta, S. Ogata, S. Sekiguchi, Y. Tanaka, and K. Tsuruta, Journal of the Japan Society of Mechanical Engineers **108** (1043), 181-183 (2005).

267. Multimillion Atom Molecular Dynamics Simulations of Nanostructured Materials and Processes on Parallel Computers
P. Vashishta, R. K. Kalia, and A. Nakano, in *Handbook on Materials Modeling, Vol. 39*, edited by S. Yip (Springer, Berlin, Germany, 2005) sec. 2.25.

268. Virtualization-aware Application Framework for Hierarchical Multiscale Simulations on a Grid
A. Nakano, R. K. Kalia, A. Sharma, and P. Vashishta, in *Computational Methods in Large Scale Simulation*, edited by K. Y. Lam and H. P. Lee (World Scientific, Singapore, 2005), pp. 229-243.

269. Molecular dynamics simulations of shock propagation in high strength ceramics
R. K. Kalia, A. Nakano, and P. Vashishta *dod_ugc*, pp. 240-243, 2005 Users Group Conference (DOD-UGC'05), 2005.

270. Virtualization-aware application framework for hierarchical multiscale simulations on a Grid (invited contribution)
A. Nakano, R. K. Kalia, A. Sharma, and P. Vashishta, in Computational Methods in Large Scale Simulation, edited by K. Y. Lam and H. P. Lee (World Scientific, Singapore, 2005), pp. 229-243.

271. Sustainable adaptive Grid supercomputing: multiscale simulation of semiconductor processing across the Pacific
H. Takemiya, Y. Tanaka, S. Sekiguchi, S. Ogata, R. K. Kalia, A. Nakano, and P. Vashishta in Proceedings of Supercomputing 2006 (IEEE Computer Society, Los Alamitos, CA, 2006).

272. Shock-induced structural transition, plasticity, and brittle cracks in aluminum nitride ceramic: A molecular dynamics study
P. S. Branicio, R. K. Kalia, A. Nakano, and P. Vashishta, Phys. Rev. Lett. **96**, 065502: 1-4 (2006).

273. Pressure-induced structural transformations in cadmium selenide nanorods
N. J. Lee, R. K. Kalia, A. Nakano, and P. Vashishta Applied Physics Letters **89**, 093101: 1-3 (2006).

274. Multimillion atom simulations of dynamics of oxidation of an aluminum nanoparticle and nanoindentation on ceramics
P. Vashishta R. K. Kalia, and A. Nakano Journal of Physical Chemistry **B 110**, 3727-3733 (2006).

275. A perspective on modeling materials in extreme environments: oxidation of ultra-high temperature ceramics
A. Bongiorno, C. Foerst, R. K. Kalia, J. Li, J. Marschall, A. Nakano, M. M. Opeka, I. G. Talmy, P. Vashishta, and S. Yip Materials Research Society Bulletin **31**, 410-418 (2006).

276. Collision-free spatial hash functions for structural analysis of billion-vertex chemical bond networks
C. Zhang, B. Bansal, P. S. Branicio, R. K. Kalia, A. Nakano, A. Sharma, and P. Vashishta Computer Physics Communications **175**, 339-347 (2006).

277. RDX (1,3,5-trinitro-1,3,5-triazine) decomposition and chemisorption on Al(111) surface: First-principles molecular dynamics study
N. Umezawa, R. K. Kalia, A. Nakano, and P. Vashishta, J Chem. Phys. **126**, 234702 (2007).

278. Adaptive Grid-enabled SIMOX simulation on Japan-US Grid testbed
Y. Tanaka, H. Takemiya, S. Sekiguchi, S. Ogata, R. K. Kalia, A. Nakano, and P. Vashishta in Proceedings of 2006 TeraGrid Conference (Indianapolis, IN, June 12-15, 2006).

279. A divide-and-conquer/cellular-decomposition framework for million-to-billion atom simulations of chemical reactions
A. Nakano, R. K. Kalia, K. Nomura, A. Sharma, P. Vashishta, F. Shimojo, A. C. T. van Duin, W. A. Goddard, III, R. Biswas, and D. Srivastava, *Computational Materials Science* **38**, 642-652 (2007).

280. Parallel history matching and associated forecast at the Center for Interactive Smart Oilfield Technologies
K. Nomura, R. K. Kalia, A. Nakano, P. Vashishta, and J. L. Landa, *Journal of Supercomputing* **41**, 109-117 (2007).

281. ParaViz: a spatially decomposed parallel visualization algorithm using hierarchical visibility ordering
C. Zhang, S. Callaghan, T. Jordan, R. K. Kalia, A. Nakano, and P. Vashishta, *International Journal of Computational Science* **1**, 407-421 (2007).

282. Interaction potential for silicon carbide: a molecular dynamics study of elastic constants and vibrational density of states for crystalline and amorphous silicon carbide
P. Vashishta, R. K. Kalia, A. Nakano, and J. P. Rino, *Journal of Applied Physics* **101**, 103515: 1-12 (2007).

283. 1,3,5-trinitro-1,3,5-triazine decomposition and chemisorption on Al(111) surface: first-principles molecular dynamics study
N. Umezawa, R. K. Kalia, A. Nakano, P. Vashishta, and F. Shimojo, *Journal of Chemical Physics* **126**, 234702: 1-7 (2007).

284. Multimillion atom simulations of dynamics of wing cracks and nanoscale damage in glass, and hypervelocity impact damage in ceramics
P. Vashishta, R. K. Kalia, and A. Nakano, *Computer Physics Communications* **177**, 202-205 (2007).

285. Multimillion atom reactive simulations of nanostructured energetic materials
P. Vashishta, R. K. Kalia, A. Nakano, B. E. Homan, and K. L. McNesby, *Journal of Propulsion and Power* **23**, 688-692 (2007).

286. A molecular dynamics study of nanoindentation of amorphous silicon carbide
I. Szlufarska, R. K. Kalia, A. Nakano, and P. Vashishta, *Journal of Applied Physics* **102**, 023509: 1-9 (2007).

287. Hypervelocity impact induced deformation modes in α-alumina
C. Zhang, R. K. Kalia, A. Nakano, and P. Vashishta, *Applied Physics Letters* **91**, 071906: 1-3 (2007)

288. Fracture initiation mechanisms in α-alumina under hypervelocity impact
C. Zhang, R. K. Kalia, A. Nakano, and P. Vashishta, *Applied Physics Letters* **91**, 121911: 1-3 (2007).

289. Multimillion-atom nanoindentation simulation of crystalline silicon carbide: orientation dependence and anisotropic pileup
H. Chen, R. K. Kalia, A. Nakano, P. Vashishta, and I. Szlufarska, *Journal of Applied Physics* **102**, 063514: 1-9 (2007).

290. Dynamic transition in the structure of an energetic crystal during chemical reactions at shock front prior to detonation
K. Nomura, R. K. Kalia, A. Nakano, P. Vashishta, A. C. T. van Duin, and W. A. Goddard III, *Physical Review Letters* **99**, 148303: 1-4 (2007).

291. Interaction of voids and nanoductility in silica glass
Y. Chen, Z. Lu, K. Nomura, W. Wang, R. K. Kalia, A. Nakano, and P. Vashishta, *Physical Review Letters* **99**, 155506: 1-4 (2007).

292. Reactive nanojets: nanostructure-enhanced chemical reactions in a defected energetic crystal
K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta, *Applied Physics Letters* **91**, 183109: 1-3 (2007).

293. Multimillion-atom nanoindentation simulation of crystalline silicon carbide: orientation dependence and anisotropic pileup
H. Chen, A. Nakano, R. K. Kalia, P. Vashishta, and I. Szlufarska, *Materials Research Society Symposium Proceedings* **1021**, HH03-08: 1-6 (2007).

294. Molecular dynamic simulation of nanoindentation of cyclotrimethylenetrintramine (RDX) crystal
Y. Chen, A. Nakano, R. K. Kalia, K. Nomura, and P. Vashishta, *Materials Research Society Symposium Proceedings* **1021**, HH03-09: 1-5 (2007).

295. Hyper velocity impact damage in alpha-alumina
C. Zhang, A. Nakano, R. K. Kalia, and P. Vashishta, *Materials Research Society Symposium Proceedings* **1021**, HH03-10: 1-7 (2007).

296. Nanoscale thermal property of amorphous SiC: a molecular dynamics study
W. Wang, A. Nakano, R. K. Kalia, and P. Vashishta, *Materials Research Society Symposium Proceedings* **1022**, II05-10: 1-6 (2007).

297. A scalable parallel algorithm for large-scale reactive force-field molecular dynamics simulations
K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta, *Computer Physics Communications* **178**, 73-87 (2008).

298. De novo ultrascale atomistic simulations on high-end parallel supercomputers
A. Nakano, R. K. Kalia, K. Nomura, A. Sharma, P. Vashishta, F. Shimojo, A. C. T. van Duin, W. A. Goddard, III, R. Biswas, D. Srivastava, and L. H. Yang
International Journal of High Performance Computing Applications **22**, 113-128 (2008).

299. Parallel lattice Boltzmann flow simulation on a low-cost PlayStation3 cluster
K. Nomura, S. W. de Leeuw, R. K. Kalia, A. Nakano, L. Peng, R. Seymour, L. H. Yang, and P. Vashishta
International Journal of Computational Science **2**, 437-449 (2008).

300. Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina
P. Vashishta, R. K. Kalia, A. Nakano, and J. P. Rino
Journal of Applied Physics **103**, 083504: 1-13 (2008).

301. Atomistic damage mechanisms during hypervelocity projectile impact on AlN: a large-scale parallel molecular dynamics simulation study
P. S. Branicio, R. K. Kalia, A. Nakano, P. Vashishtaa, F. Shimojoc, and J. P. Rino
Journal of the Mechanics and Physics of Solids **56**, 1955-1988 (2008).

302. Deformations and failure of α-alumina under hypervelocity impact loading
C. Zhang, P. S. Branicio, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Applied Physics **103**, 083508: 1-15 (2008).

303. Nanoindentation hardness anisotropy of alumina crystal: a molecular-dynamics study
K. Nishimura, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letters **92**, 161904: 1-3 (2008).

304. Electronic processes in fast thermite reaction: a first-principles molecular dynamics study
F. Shimojo, A. Nakano, R. K. Kalia, and P. Vashishta
Physical Review E **77**, 066103: 1-7 (2008).

305. Metascalable molecular dynamics simulation of nano-mechano-chemistry
F. Shimojo, R. K. Kalia, A. Nakano, K. Nomura, and P. Vashishta
Journal of Physics: Condensed Matter **20**, 294204: 1-9 (2008).

306. Molecular dynamics nanoindentation simulation of an energetic materials
Y. Chen, K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letters **93**, 171908: 1-2 (2008).

307. Divide-and-conquer density functional theory on hierarchical real-space grids: parallel implementation and applications
F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Physical Review B **77**, 085103:1-12 (2008).

308. A scalable parallel algorithm for large-scale reactive force-field molecular dynamics simulations
K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta
Computer Physics Communications **178**, 73-87 (2008).

309. Hierarchical petascale simulation framework for stress corrosion cracking
P. Vashishta, R. K. Kalia, A. Nakano, E. Kaxiras, A. Grama, G. Lu, S. Eidenbenz, A. F. Voter, R. Q. Hood, J. A. Moriarty, and L. H. Yang
Journal of Physics: Conference Series **125** 012060: 1-18 (2008).

310. Parallel lattice Boltzmann flow simulation on emerging multi-core platforms
L. Peng, K. Nomura, T. Oyakawa, R. K. Kalia, A. Nakano, and P. Vashishta
Lecture Notes in Computer Science **5168**, 763-777 (2008); *Proceedings of the 14th International European Conference on Parallel and Distributed Computing, Euro-Par 2008* (Las Palmas de Gran Canaria, Spain, August 26-29, 2008) pp. 763-777.

311. Large spatiotemporal-scale material simulations on petaflops computers
K. Nomura, W. Wang, R. K. Kalia, A. Nakano, P. Vashishta, and F. Shimojo, in *Multiscale Simulation Methods in Molecular Sciences*, edited by J. Grotendorst, N. Attig, S. Blügel, and D. Marx (John von Neumann Institut für Computing, Jülich, Germany, 2009) pp. 321-336.

312. An MPI performance monitoring interface for cell based compute nodes
H. Dursun, K. J. Barker, D. J. Kerbyson, S. Pakin, R. Seymour, R. K. Kalia, A. Nakano, and P. Vashishta
Parallel Processing Letters **19**, 535-552 (2009).

313. Molecular dynamical approach to conformational transition in peptide nanoring and nanotube
M. Teranishi, H. Okamoto, K. Takeda, K. Nomura, A. Nakano, R. K. Kalia, P. Vashishta, and F. Shimojo
Journal of Physical Chemistry B **113**, 1473-1484 (2009).

314. Response to "Comment of 'Nanoindentation hardness anisotropy of alumina crystal: a molecular-dynamics study'" [Appl. Phys. Lett. 94, 146101 (2009)]
K. Nishimura, H. Chen, R. K. Kalia, A. Nakano, K. Nomura, P. Vashishta, and F. Shimojo
Applied Physics Letters **94**, 146102: 1-2 (2009).

315. Erratum: "Molecular dynamics simulation studies of amorphous and liquid alumina" [J. Appl. Phys. 103, 083504 (2008)]
P. Vashishta, R. K. Kalia, A. Nakano, and J. P. Rino
Journal of Applied Physics **105**, 059901: 1-1 (2009).

316. Void deformation and breakup in shearing silica glass
Y. Chen, K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta
Physical Review Letters **103**, 035501: 1-4 (2009).

317. Enhanced reactivity of nanoenergetic materials: a first-principles molecular dynamics study based on divide-and-conquer density functional theory
F. Shimojo, A. Nakano, R. K. Kalia, and P. Vashishta
Applied Physics Letters **95**, 043114: 1-3 (2009).

318. Interaction and coalescence of nanovoids and dynamic fracture in silica glass: multimillion-to-billion atom molecular dynamics simulations
K. Nomura, Y. Chen, W. Wang, R. K Kalia, A. Nakano, P. Vashishta, and L. H Yang
Journal of Physics D **42**, 214011: 1-12 (2009).

319. Fast reaction mechanism of a core (Al)-shell (Al_2O_3) nanoparticle in oxygen
W. Wang, R. Clark, A. Nakano, R. K. Kalia, and P. Vashishta
Applied Physics Letters **95**, 261901: 1-3 (2009).

320. A metascalable computing framework for large spatiotemporal-scale atomistic simulations
K. Nomura, H. Dursun, R. Seymour, W. Wang, R. K. Kalia, A. Nakano, P. Vashishta, F. Shimojo, and L. H. Yang, in *Proceedings of the 2009 International Parallel and Distributed Processing Symposium* (IEEE, Rome, Italy, 2009).

321. High-order stencil computations on multicore clusters
L. Peng, R. Seymour, K. Nomura, R. K. Kalia, A. Nakano, P. Vashishta, A. Loddoch, M. Netzband, W. R. Volz, and C. C. Wong, in *Proceedings of the 2009 International Parallel and Distributed Processing Symposium* (IEEE, Rome, Italy, 2009).

322. A scalable hierarchical parallelization framework for molecular dynamics simulation on multicore clusters
L. Peng, M. Kunaseth, H. Dursun, K. Nomura, W. Wang, R. K. Kalia, A. Nakano, and P. Vashishta, in *Proceedings of the International Conference on Parallel and Distributed Processing Techniques and Applications* (Las Vegas, NV, 2009).

323. In-core optimization of high-order stencil computations
H. Dursun, K. Nomura, W. Wang, M. Kunaseth, L. Peng, R. Seymour, R. K. Kalia, A. Nakano, and P. Vashishta, in *Proceedings of the International Conference on Parallel and Distributed Processing Techniques and Applications* (Las Vegas, NV, 2009).

324. A multilevel parallelization framework for high-order stencil computations
H. Dursun, K. Nomura, L. Peng, R. Seymour, W. Wang, R. K. Kalia, A. Nakano, and P. Vashishta, in *International European Conference on Parallel and Distributed Computing, Euro-Par 2009* (Delft, The Netherlands, August 25-28, 2009).

325. Multi-million atom molecular dynamics study of combustion mechanism of aluminum nanoparticle
W. Wang, R. Clark, A. Nakano, R. K. Kalia, and P. Vashishta
Materials Research Society Symposium Proceedings **1137**, EE-10-29: 1-6 (2009).

326. DNA sequencing via quantum mechanics and machine learning
H. Yuen, F. Shimojo, K. J. Zhang, K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta
International Journal of Computational Science **4**, 352-370 (2010) .

327. Nanoductility induced brittle fracture in shocked high performance ceramics
P. S. Branicio, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letters **97**, 111903: 1-3 (2010) .

328. Performance modeling, analysis, and optimization of cell-list based molecular dynamics
M. Kunaseth, R. K. Kalia, A. Nakano, and P. Vashishta
Proceeding of International Conference on Scientific Computing (2010).

329. Structure and dynamics of shock-induced nanobubble collapse in water
M. Vedadi, A. Choubey, K. Nomura, R. K. Kalia, A. Nakano, P. Vashishta, and A. C. T. van Duin
Physical Review Letters **105**, 014503: 1-4 (2010).

330. Effects of oxide-shell structures on the dynamics of oxidation of Al nanoparticle
W. Wang, R. Clark, A. Nakano, R. K. Kalia, and P. Vashishta
Applied Physics Letters **96**, 181906: 1-3 (2010).

331. Embrittlement of metal by solute segregation-induced amorphization
H. Chen, R. K. Kalia, E. Kaxiras, G. Lu, A. Nakano, K. Nomura, A. C. T. van Duin, P. Vashishta, and Z. Yuan
Physical Review Letters **104**, 155502: 1-4 (2010).

332. Molecular dynamics simulations of rapid hydrogen production from water using aluminum clusters as catalyzers
F. Shimojo, S. Ohmura, R. K. Kalia, A. Nakano, and P. Vashishta
Physical Review Letters **104**, 126102: 1-4 (2010).

333. Density functional study of 1,3,5-trinitro-1,3,5-triazine molecular crystal with van der Waals interaction
F. Shimojo, Z. Wu, A. Nakano, R. K. Kalia, and P. Vashishta
Journal of Chemical Physics **132**, 094106: 1-8 (2010).

334. Effects of solvation shells and cluster size on the reaction of aluminum clusters with water
W. Mou, S. Ohmura, A. Hemeryck, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
AIP Advances **1**, 042149: 1-13 (2011).

335. Sulfur-impurity induced amorphization of nickel
Z. Yuan, H.-P. Chen, W. Wang, K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Applied Physics **110**, 063501: 1-6 (2011).

336. Defect migration and recombination in nanoindentation of silica glass
K. Nomura, Y. Chen, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letters **99**, 111906: 1-3 (2011).

337. Exploiting hierarchical parallelisms for molecular dynamics simulation on multicore clusters
L. Peng, M. Kunaseth, H. Dursun, K. Nomura, W. Wang, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Supercomputing **57**, 20-33 (2011).

338. Scalable data-privatization threading for hybrid MPI/OpenMP parallelization of molecular dynamic
M. Kunaseth, D. F. Richards, J. N. Glosli, R. K. Kalia, A. Nakano, and P. Vashishta
Proceeding of International Conference on Parallel and Distributed Processing Techniques and Applications (2011).

339. Reaction of aluminum clusters with water
S. Ohmura, F. Shimojo, R. K. Kalia, M. Kunaseth, A. Nakano, and P. Vashishta
Journal of Chemical Physics **134**, 244702: 1-8 (2011).

340. Vibrational and thermodynamic properties of β-HMX: a first-principles investigation
Z. Wu, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Chemical Physics **134**, 204509: 1-10 (2011).

341. First-principles calculations of the structural and dynamic properties, and the equation of state of crystalline iodine oxides I_2O_4, I_2O_5, and I_2O_6
Z. Wu, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Chemical Physics **134**, 204501: 1-14 (2011).

342. Atomistic mechanisms of rapid energy transport in light-harvesting molecules
S. Ohmura, S. Koga, I. Akai, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letters **98**, 113302: 1-3 (2011).

343. Interaction potential for aluminum nitride: a molecular dynamics study of mechanical and thermal properties of crystalline and amorphous aluminum nitride
P. Vashishta, R. K. Kalia, A. Nakano, and J. P. Rino
Journal of Applied Physics **109**, 033514: 1-8 (2011).

344. Poration of lipid bilayers by shock-induced nanobubble collapse
A. Choubey, M. Vedadi, K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letters **98**, 023701: 1-3 (2011).

345. Heat-initiated oxidation of an aluminum nanoparticle_
R. Clark, W. Wang, K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta
Materials Research Society Symposium Proceedings **1405**, Y-08-07: 1-7 (2012).

346. Hierarchical parallelization and optimization of high-order stencil computations on multicore clusters_
H. Dursun, M. Kunaseth, K. Nomura, J. Chame, R. F. Lucas, C. Chen, M. Hall, R. K. Kalia, A. Nakano, and P. Vashishta, *Journal of Supercomputing* **62**, 946-966 (2012).

347. Molecular mechanism of flip-flop in triple-layer oleic-acid membrane: correlation between oleic acid and water
V. Ngo, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Physical Chemistry B 116, 13416–13423 (2012).

348. Supercrystals of DNA-functionalized gold nanoparticles: a million-atom molecular dynamics simulation study
V. Ngo, R. K. Kalia, A. Nakano, and P. Vashishta, Journal of Physical Chemistry C 116, 19579-19585 (2012).

349. Large nonadiabatic quantum molecular dynamics simulations on parallel computers
F. Shimojo, S. Ohmura, W. Mou, R. K. Kalia, A. Nakano, and P. Vashishta, *Computer Physics Communications* **184**, 1-8 (2013).

350. Hierarchical parallelization and optimization of high-order stencil computations on multicore clusters
H. Dursun, M. Kunaseth, K. Nomura, J. Chame, R. F. Lucas, C. Chen, M. Hall, R. K. Kalia, A. Nakano, P. Vashishta, *Journal of Supercomputing* **62**, 946-966 (2012).

351. Memory-access optimization of parallel molecular dynamics simulation via dynamic data reordering
M. Kunaseth, K. Nomura, H. Dursun, R. K. Kalia, A. Nakano, P. Vashishta, *Proceedings of the International Euro-Par Conference on Parallel Processing* **7484**, 781-792 (2012).

352. Mechanochemistry of shock-induced nanobubble collapse near silica in water
K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta, *Applied Physics Letters* **101**, 073108: 1-4 (2012).

353. Ion dynamics at porous alumina surfaces
S. Hattori, R. K. Kalia, A. Nakano, K. Nomura, and P. Vashishta, *Applied Physics Letters* **101**, 063106: 1-4 (2012).

354. Cholesterol translocation in a phospholipid membrane
Amit Choubey, Rajiv K. Kalia, Noah Malmstadt, Aiichiro Nakano, Priya Vashishta, *Biophysical Journal* **104**, 2429–2436 (2013).

355. Nanobubble collapse on silica surface – billion-atom reactive molecular dynamics simulations on the IBM BlueGene/P
Adarsh Shekhar, Ken-ichi Nomura, Rajiv K. Kalia, Aiichiro Nakano and Priya Vashishta, *Physical Review Letters* **111**, 1845031- 1845035 (2013).

356. Performance characteristics of hardware transactional memory for molecular dynamics application on BlueGene/Q: Toward efficient multithreading strategies for large-scale scientific applications (Best Paper Award of IEEE-PDSEC13)
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).

357. 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).

358. 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).

359. 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).

360. 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).

361. 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).

362. 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).

363. 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).

364. 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).

365. 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).

366. 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).

367. 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).

368. 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).

369. 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).

370. Twin superlattice-induced large surface recombination velocity in GaAs nanostructures
C. Sheng, E. Brown, F. Shimojo, and A. Nakano
Applied Physics Letters **105**, 231602: 1-5 (2014).

371. Metascalable quantum molecular dynamics simulations of hydrogen-on-demand
K. Nomura, R. K. Kalia, A. Nakano, P. Vashishta, K. Shimamura, F. Shimojo, M. Kunaseth, P. C. Messina, and N. A. Romero
Proceedings of Supercomputing **SC14**, 661-673 (2014).

372. An extended-Lagrangian scheme for charge equilibration in reactive molecular dynamics simulations
K. Nomura, P. E. Small, R. K. Kalia, A. Nakano, and P. Vashishta
Computer Physics Communications **192**, 91-96 (2015).

373. Reactive molecular dynamics simulations, data analytics and visualization
P. Vashishta, R. K. Kalia, A. Nakano, Y. Li, K. Nomura, A. Shekhar, F. Shimojo, K. Shimamura, and M. Kunaseth
Materials Research Society Symposium Proceedings **1756**, SS06-01: 1-12 (2015).

374. Quantum molecular dynamics in the post-petaflop/s era
N. A. Romero, A. Nakano, K. Riley, F. Shimojo, R. K. Kalia, P. Vashishta, P. C. Messina
IEEE Computer, **48**, 33-41 (2015).

375. Oxidation dynamics of aluminum nanorods
Y. Li, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letters **106**, 083101: 1-5 (2015).

376. Enhanced charge recombination due to surfaces and twin defects in GaAs nanostructures
E. Brown, C. Sheng, K. Shimamura, F. Shimojo, and A. Nakano
Journal of Applied Physics **117**, 054307: 1-8 (2015).

377. Dynamics of supercooled water in nanotubes: Cage correlation function and diffusion coefficient
M. Khademi, R. K. Kalia, M. Sahimi
Physical Review ***E*** **92**, 030301(R) (2015).

378. Vibrational and thermodynamic properties of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB): comparison of exchange-correlation functionals in density functional theory
Z. Wu, W. Mou, R. K. Kalia, A. Nakano, and P. Vashishta
International Journal of Energetic Materials and Chemical Propulsion **14**, 519–547 (2015).

379. A crossover in anisotropic nanomechanochemistry of van der Waals crystals
K. Shimamura, M. Misawa, Y. Li, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta
Applied Physics Letters **107**, 231903: 1-5 (2015).

380. Reactive molecular dynamics study of oxidation of aggregated aluminum nanoparticles
Y. Li, R. K. Kalia, A. Nakano, and P. Vashishta
Materials Research Society Symposium Proceedings **1758**, VV03-03: 1-6 (2015).

381. First-principles study of the adsorption/dissociation reactions of water on a Fe- and Co-Al_2O_4 cluster
M. Misawa, A. Koura, F. Shimojo, R. K. Kalia, A. Nakano and P. Vashishta
e-Journal of Surface Science and Nanotechnology **13**, 410-412 (2015).

382. Divide-conquer-recombine: an algorithmic pathway toward metascalability
A. Nakano, S. Hattori, R. K. Kalia, W. Mou, K. Nomura, P. Rajak, P. Vashishta, K. Shimamura, F. Shimojo, M. Kunaseth, S. Ohmura, P. C. Messina, and N. A. Romero
i*Proceedings of Beowulf 14* (ACM, New York, NY, 2015) pp. 17-27.

383. Rotation mechanism of methylammonium molecules in organometal halide perovskite in cubic phase: an *ab initio* molecular dynamics study
K. Shimamura, T. Hakamata, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Chemical Physics **145**, 224503: 1-19 (2016).

384. Anisotropic mechanochemistry of energetic van der Waals crystallites: an *ab initio* nanocollider study
Y. Li, R. K. Kalia, M. Misawa, A. Nakano, K. Nomura, K. Shimamura, F. Shimojo, and P. Vashishta
Nanoscale **8**, 9714-9720 (2016).

385. Nanocarbon synthesis by high-temperature oxidation of nanoparticles
K. Nomura, R. K. Kalia, Y. Li, A. Nakano, P. Rajak, C. Sheng, K. Shimamura, F. Shimojo, and P. Vashishta
Scientific Reports **6**, 24109: 1-7 (2016).

386. The nature of free-carrier transport in organometal halide perovskites
T. Hakamata, K. Shimamura, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Scientific Reports **5**, 19599: 1-6 (2016).

387. Crystalline anisotropy of shock-induced phenomena: omni-directional multiscale shock technique
K. Shimamura, M. Misawa, S. Ohmura, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letters **108**, 071901: 1-5 (2016).

388. Shock induced decomposition of TATB: a ReaxFF molecular dynamics study
S. C. Tiwari, K. Nomura, R. K. Kalia, A. Nakano and P. Vashishta
MRS Advances **1**, 1247-1253 (2016).

389. Quantum molecular dynamics validation of nanocarbon synthesis by high-temperature oxidation of nanoparticles
C. Sheng, K. Nomura, P. Rajak, A. Nakano, R. K. Kalia, and P. Vashishta
MRS Advances **1**, 1811-1816 (2016).

390. Order-invariant real number summation: circumventing accuracy loss for multimillion summands on multiple parallel architectures
P. E. Small, R. K. Kalia, A. Nakano, and P. Vashishta
Proceedings of the International Parallel and Distributed Processing Symposium, IPDPS 2016 (IEEE, Chicago, IL, 2016) pp. 152-160.

391. A high-throughput multiobjective genetic-algorithm workflow for *in situ* training of reactive molecular-dynamics force fields
H. C. Cheng, P. Rajak, C. Sheng, R. K. Kalia, A. Nakano, P. Vashishta, and E. Brown
Proceedings of SpringSim HPC2016 (SCS, Pasadena, CA, 2016).

392. Multiple reaction pathways in shocked 2,4,6-triamino-1,3,5-trinitrobenzene crystal
S. C. Tiwari, K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Physical Chemistry C **121**, 16029-16034 (2017).

393. Computational synthesis of MoS_2 layers by reactive molecular dynamics simulations: initial sulfidation of MoO_3 surfaces
S. Hong, A. Krishnamoorthy, P. Rajak, S. Tiwari, M. Misawa, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Nano Letters **17**, 4866-4872 (2017).

394. A derivation and scalable implementation of the synchronous parallel kinetic Monte Carlo method for simulating long-time dynamics
H. S. Byun, M. Y. El-Naggar, R. K. Kalia, A. Nakano, and P. Vashishta
Computer Physics Communications **219**, 246-254 (2017).

395. Picosecond amorphization of SiO_2 stishovite under tension
M. Misawa, E. Ryuo, K. Yoshida, R. K. Kalia, A. Nakano, N. Nishiyama, F. Shimojo, P. Vashishta, and F. Wakai
Science Advances **3**, e1602339: 1-7 (2017).

396. Re-doping in 2D transition metal dichalcogenides as a new route to tailor structural phases and induced magnetism
V. Kochat, A. Apte, J. A. Hachtel, H. Kumazoe, A. Krishnamoorthy, S. Susarla, J. C. Idrobo, F. Shimojo, P. Vashishta, R. Kalia, A. Nakano, C. S. Tiwary and P. M Ajayan
Advanced Materials **29**, 1703754: 1-8 (2017).

397. Gel phase in hydrated calcium dipicolinate
P. Rajak, A. Mishra, C. Sheng, S. Tiwari, A. Krishnamoorthy, R. K. Kalia, A. Nakano and P. Vashishta
Applied Physics Letters **111**, 213701: 1-5 (2017).

398. Reactivity of sulfur molecules on MoO3 (010) surface
M. Misawa, S. Tiwari, S. Hong, A. Krishnamoorthy, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Physical Chemistry Letters **8**, 6206-6210 (2017).

399. Analysis of killing of growing cells and dormant and germinated spores of Bacillus species by black silicon nanopillars
S. Ghosh, S. Niu, M. Yankova, M. Mecklenburg, S. M. King, J. Ravichandran, R. K. Kalia, A. Nakano, P. Vashishta, and P. Setlow
Scientific Reports **7**, 17768: 1-13 (2017).

400. Ultrafast non-radiative dynamics of atomically thin $MoSe_2$
M.-F. Lin, V. Kochat, A. Krishnamoorthy, L. Bassman, C. Weninger, Q. Zheng, X. Zhang, A. Apte, C. S. Tiwary, X. Shen, R. Li, R. K. Kalia, P. Ajayan, A. Nakano, P. Vashishta, F. Shimojo, X. Wang, D. M. Fritz, and U. Bergmann
Nature Communications **8**, 1745: 1-8 (2017).

401. *Semiconductor-metal structural phase transformation in $MoTe_2$ monolayers by electronic excitation*
A. Krishnamoorthy, L. Bassman, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta
Nanoscale **10**, 2742-2747 (2018).

402. Active learning for accelerated design of layered materials
L. Bassman, P. Rajak, R. K. Kalia, A. Nakano, F. Sha, J. Sun, D. J. Singh, M. Aykol, P. Huck, K. Persson, and P. Vashishta
NPJ Computational Materials **4**, 74: 1-9 (2018).

403. Telluride-based atomically thin layers of ternary 2D transition metal dichalcogenide alloys
A. Apte, A. Krishnamoorthy, J. A. Hachtel, S. Susarla, J. C. Idrobo, A. Nakano, R. K. Kalia, P. Vashishta, C. S. Tiwary, and P. M. Ajayan
Chemistry of Materials **30**, 7262-7268 2018).

404. Energetic performance of optically activated aluminum/graphene oxide composites
Y. Jiang, S. Deng, S. Hong, J. Zhao, S. Huang, C.-C. Wu, J. L. Gottfried, K. Nomura, Y. Li, S. Tiwari, R. K. Kalia, P. Vashishta, A. Nakano, and X. Zheng
ACS Nano **12**, 11366-11375 (2018).

405. Molecular simulation of MoS_2 exfoliation
G. Zhou, P. Rajak, S. Susarla, P. M. Ajayan, R. K. Kalia, A. Nakano, and P. Vashishta
Scientific Reports **8**, 16761: 1-9 (2018).

406. Dewetting of monolayer water and isopropanol between MoS_2 nanosheets
B. Wang, R. K. Kalia, A. Nakano, and P. Vashishta
Scientific Reports **8**, 16704: 1-6 (2018).

407. Role of H transfer in the gas-phase sulfidation process of MoO3: a quantum molecular dynamics study
C. Sheng, S. Hong, A. Krishnamoorthy, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta
Journal of Physical Chemistry Letters **9**, 6517-6523 (2018).

408. Faceting, grain growth, and crack healing in alumina
P. Rajak, R. K. Kalia, A. Nakano, and P. Vashishta
ACS Nano **12**, 9005-9010 (2018).

409. Free energy of hydration and heat capacity for calcium dipicolinate in Bacillus spore cores
A. Mishra, A. Krishnamoorthy, P. Rajak, S. Tiwari, C. Sheng, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letters **113**, 113702: 1-5 (2018).

410. Electronic origin of optically-induced sub-picosecond lattice dynamics in $MoSe_2$ monolayer
L. Bassman, A. Krishnamoorthy, H. Kumazoe, M. Misawa, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Nano Letters **18**, 4653-4658 (2018).

411. Multiobjective genetic training and uncertainty quantification of reactive force fields
A. Mishra, S. Hong, P. Rajak, C. Sheng, K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta
NPJ Computational Materials **4**, 42: 1-7 (2018).

412. Photo-induced lattice contraction in layered materials
H. Kumazoe, A. Krishnamoorthy, L. Bassman, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta
Journal of Physics: Condensed Matter **30**, 32LT02: 1-6 (2018).

413. Anisotropic frictional heating and defect generation in cyclotrimethylene-trinitramine molecular crystals
P. Rajak, A. Mishra, C. Sheng, S. Tiwari, R. K. Kalia, A. Nakano, and P. Vashishta
Applied Physics Letters **122**, 211604: 1-5 (2018).

414. Chemical vapor deposition synthesis of MoS2 layers from the direct sulfidation of MoO3 surfaces using reactive molecular dynamics simulations
S. Hong, C. Sheng, A. Krishnamoorthy, P. Rajak, S. Tiwari, K. Nomura, M. Misawa, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Physical Chemistry C **122**, 7494-7503 (2018).

415. Structural phase transformation in strained monolayer MoWSe2 alloy
A. Apte, V. Kochat, P. Rajak, A. Krishnamoorthy, P. Manimunda, J. A. Hachtel, J. C. Idrobo, S. A. S. Asif, P. Vashishta, A. Nakano, R. K. Kalia, C. S. Tiwary, and P. M. Ajayan
ACS Nano **12**, 3468-3476 (2018).

416. Plane shock loading on mono- and nano-crystalline silicon carbide
P. S. Branicio, J. Zhang, J. P. Rino, A. Nakano, R. K. Kalia, and P. Vashishta
Applied Physics Letters **112**, 111909: 1-5 (2018).

417. Shock-induced microstructural response of mono- and nanocrystalline SiC ceramics
P. S. Branicio, J. Zhang, J. P. Rino, A. Nakano, R. K. Kalia, and P. Vashishta
Journal of Applied Physics **123**, 145902: 1-11 (2018).

418. Structure and dynamics of water confined in nanoporous carbon
Yuzi He, Ken-ichi Nomura, Rajiv K. Kalia, Aiichiro Nakano, and Priya Vashishta
Phys. Rev. Materials 2, 115605 (2018).

419. Guidelines for creating artificial neural network empirical interatomic potential from first-principles molecular dynamics data under specific conditions and its application to alpha-Ag_2Se
K. Shimamura, S. Fukushima, A. Koura, F. Shimojo, M. Misawa, R. K. Kalia, A. Nakano, P. Vashishta, T. Matsubara, and S. Tanaka
Journal of Chemical Physics **151**, 124303:1-10 (2019).

420. Optical control of non-equilibrium phonon dynamics
A. Krishnamoorthy, M.-F. Lin, X. Zhang, C. Weninger, R. Ma, A. Britz, C. S. Tiwary, V. Kochat, A. Apte, J. Yang, S. Park, R. Li, X. Shen, X. Wang, R. K. Kalia, A. Nakano, F. Shimojo, D. Fritz, U. Bergmann, P. Ajayan, and P. Vashishta
Nano Letters **19**, 4981-4989 (2019).

421. Scalable reactive molecular dynamics simulations for computational synthesis
Y. Li, K. Nomura, J. Insley, V. Morozov, K. Kumaran, N. A. Romero, W. A. Goddard III, R. K. Kalia, A. Nakano, and P. Vashishta
IEEE Computing in Science and Engineering **21(5)**, 64-75 (2019).

422. QXMD: an open-source program for nonadiabatic quantum molecular dynamics
F. Shimojo, S. Fukushima, H. Kumazoe, M. Misawa, S. Ohmura, P. Rajak, K. Shimamura, L. Bassman, S. Tiwari, R. K. Kalia, A. Nakano, and P. Vashishta
SoftwareX **10**, 100307: 1-5 (2019).

423. Structural phase transitions in $MoWSe_2$ monolayer - molecular dynamics simulations and variational autoencoder analysis
P. Rajak, A. Krishnamoorthy, A. Nakano, P. Vashishta, and R. K. Kalia
Physical Review B **100**, 014108: 1-7 (2019).

424. Hot-carrier dynamics and chemistry in dielectric polymers
H. Kumazoe, S. Fukushima, S. C. Tiwari, C. Kim, H. Tran, R. K. Kalia, A. Nakano, R. Ramprasad, F. Shimojo, and P. Vashishta
Journal of Physical Chemistry Letters **10**, 3937-3943 (2019).

425. Anisotropic structural dynamics of monolayer crystals revealed by femtosecond surface x-ray scattering
I. Tung, A. Krishnamoorthy, S. Sadasivam, H. Zhou, Q. Zhang, K. L. Seyler, G. Clark, E. M. Mannebach, C. Nyby, F. Ernst, D. Zhu, J. M. Glownia, M. E. Kozina, S. Song, S. Nelson, H. Kumazoe, F. Shimojo, R. K. Kalia, P. Vashishta, P. Darancet, T. F. Heinz, A. Nakano, X. Xu, A. M. Lindenberg, and H. Wen
Nature Photonics **13**, 425-430 (2019).

426. Nanoindentation on monolayer MoS_2 kirigami
B. Wang, A. Nakano, P. Vashishta, and R. K. Kalia
ACS Omega **4**, 9952-9956 (2019).

427. Defect healing in layered materials: a machine learning-assisted characterization of MoS_2 crystal-phases
S. Hong, K. Nomura, A. Krishnamoorthy, P. Rajak, C. Sheng, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Physical Chemistry Letters **10**, 2739-2744 (2019).

428. Effects of chemical defects on anisotropic dielectric response of polyethylene
S. Fukushima, S. Tiwari, H. Kumazoe, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta
AIP Advances **9**, 045022: 1-5 (2019).

429. Thermal conductivity of MoS_2 monolayers from molecular dynamics simulations
A. Krishnamoorthy, P. Rajak, N. Payam, D. J. Singh, R. K. Kalia, A. Nakano, and P. Vashishta
AIP Advances **9**, 035042: 1-6 (2019).

430. Rapid and reversible lithiation of doped biogenous iron oxide nanoparticles
M. Misawa, H. Hashimoto, R. K. Kalia, S. Matsumoto, A. Nakano, F. Shimojo, J. Takada, S. Tiwari, K. Tsuruta, and P. Vashishta
Scientific Reports **9**, 1828: 1-8 (2019).

431. Game-Engine-Assisted Research platform for Scientific computing (GEARS) in virtual reality
B. K. Horton, R. K. Kalia, E. Moen, A. Nakano, K. Nomura, M. Qian, P. Vashishta, and A. Hafreager
SoftwareX **9**, 112-116 (2019).

432. Polytypism in ultrathin tellurium
A. Apte, E. Bianco, A. Krishnamoorthy, S. Yazdi, R. N. Glavin, H. Kumazoe, V. Varshney, A. Roy, F. Shimojo, E. Ringe, R. K. Kalia, A. Nakano, C. Tiwary, P. Vashishta, V. Kochat, and P. M. Ajayan
2D Materials **6**, 015013: 1-10 (2019).

433. Electrostrictive cavitation in water induced by a SnO_2 nanoparticle
S. Jackson, A. Nakano, P. Vashishta, and R. K. Kalia
ACS Omega **4**, 22274-22279 (2019).

434. Thermodynamic integration by neural network potentials based on first-principles dynamic calculations
S. Fukushima, E. Ushijima, H. Kumazoe, A. Koura, F. Shimojo, K. Shimamura, M. Misawa, R. K. Kalia, A. Nakano, and P. Vashishta
Physical Review B **100**, 214108:1-8 (2019).

435. Hydrogen bond preserving shock release mechanism is key to the resilience of aramid fibers
S. C. Tiwari, K. Shimamura, A. Mishra, F. Shimojo, A. Nakano, R. K. Kalia, P. Vashishta, and P. S. Branicio
Journal of Physical Chemistry B **123**, 9719-9723 (2019).

436. Atomistic simulations of biofouling and molecular transfer of crosslinked aromatic polyamide membrane for desalination
M. S. J. Sajib, Y. Wei, A. Mishra, L. Zhang, K. Nomura, R. K. Kalia, P. Vashishta, A. Nakano, S. Murad, and T. Wei
Langmuir **36**, 7658-7668 (2020).

437. Enhancing combustion performance of nano-Al/PVDF composites with beta-PVDF
S. Huang, S. Hong, Y. Su, Y. Jiang, S. Fukushima, T. M. Gill, N. E. D. Yilmaz, S. C. Tiwari, K. Nomura, R. K. Kalia, A. Nakano, F. Shimojo, P. Vashishta, M. Chen, and X. Zheng
Combustion and Flame **219**, 467-477 (2020).

438. Memristive device characteristics engineering by controlling the crystallinity of switching layer material
H. Yang, B. Chen, B. Song, D. Meng, S. C. Tiwari, A. Krishnamoorthy, X. Yan, Z. Liu, Y. Wang, P. Hu, T. Ou, P. S. Branicio, R. K. Kalia, A. Nakano, P. Vashishta, F. Liu, H. Wang, and W. Wu
Applied Electronic Materials **2**, 1529-1537 (2020).

439. Application of first-principles-based artificial neural network potentials to multiscale-shock dynamics simulations on solid materials
M. Misawa, S. Fukushima, A. Koura, K. Shimamura, F. Shimojo, S. C. Tiwari, K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Physical Chemistry Letters **11**, 4536-4541 (2020).

440. Towards dynamic simulations of materials on quantum computers
L. Bassman, K. Liu, A. Krishnamoorthy, T. Linker, Y. Geng, D. Shebib, S. Fukushima, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Physical Review B **101**, 184305: 1-6 (2020).

441. Evolutionary multi-objective optimization and Pareto-frontal uncertainty quantification of interatomic forcefields for thermal conductivity simulations
A. Krishnamoorthy, A. Mishra, N. Grabar, N. Baradwaj, R. K. Kalia, A. Nakano, and P. Vashishta
Computer Physics Communications **254**, 107337: 1-7 (2020).

442. Direct atomic simulations of facet formation and equilibrium shapes of SiC nanoparticles
H. A. Sveinsson, A. Hafreager, R. K. Kalia, A. Nakano, P. Vashishta, and A. Malthe-Sorenssen
Crystal Growth & Design **20**, 2147-2152 (2020).

443. Fluidic flow assisted deterministic folding of van der Waals materials
H. Zhao, B. Wang, F. Liu, X. Yan, H. Wang, M. J. Stevens, P. Vashishta, A. Nakano, J. Kong, R. K. Kalia, and H. Wang
Advanced Functional Materials **30**, 1908691: 1-7 (2020).

444. Synergistically chemical and thermal coupling between graphene oxide and graphene fluoride for enhancing aluminum combustion
Y. Jiang, S. Deng, S. Hong, S. C. Tiwari, H. Chen, K. Nomura, R. K. Kalia, A. Nakano, P. Vashishta, M. R. Zachariah, and X. Zheng
ACS Applied Materials & Interfaces **12**, 7451-7458 (2020).

445. Quantum dynamics at scale: ultrafast control of emergent functional materials
S. C. Tiwari, P. Sakdhnagool, R. K. Kalia, A. Krishnamoorthy, M. Kunaseth, A. Nakano, K. Nomura, P. Rajak, F. Shimojo, Y. Luo, and P. Vashishta
Proceedings of International Conference on High Performance Computing in Asia-Pacific Region, HPCAsia2020 **best paper award**, 1-10 (2020).

446. Field-induced carrier localization transition in dielectric polymers
T. M. Linker, S. C. Tiwari, H. Kumazoe, S. Fukushima, R. K. Kalia, A. Nakano, R. Ramprasad, F. Shimojo, and P. Vashishta
Journal of Physical Chemistry Letters **11**, 352-358 (2020).

447. RXMD: a scalable reactive molecular dynamics simulator for optimized time-to-solution
K. Nomura, R. K. Kalia, A. Nakano, P. Rajak, and P. Vashishta
SoftwareX **11**, 100389:1-6 (2020).

448. Boltzmann machine modeling of layered MoS_2 synthesis on a quantum annealer
J. Liu, A. Mohan, K. Nomura, A. Nakano, P. Vashishta, K. Yao, and R. K. Kalia
Computational Materials Science **173**, 109429:1-5 (2020).

449. Photoexcitation induced ultrafast nonthermal amorphization in Sb_2Te_3
S. C. Tiwari, R. K. Kalia, A. Nakano, F. Shimojo, P. Vashishta, and P. S. Branicio
Journal of Physical Chemistry Letters **11**, 10242-10249 (2020).

450. Optically induced three-stage picosecond amorphization in low temperature $SrTiO_3$
T. Linker, S. Tiwari, S. Fukushima, R. K. Kalia, A. Krishnamoorthy, A. Nakano, K. Nomura, K. Shimamura, F. Shimojo, and P. Vashishta
Journal of Physical Chemistry Letters **11**, 9605-9612 (2020).

451. Differences in Sb_2Te_3 growth by pulsed laser and sputter deposition
J. Ning, J. C. Martinez, J. Momand, H. Zhang, S. C. Tiwari, F. Shimojo, A. Nakano, R. K. Kalia, P. Vashishta, P. S. Branicio, B. J. Kooi, and R. E. Simpson
Acta Materialia **200**, 811-820 (2020).

452. Tape-time processing: kinetics and mechanisms of native oxidation of transition metal dichalcogenides $ZrSxSe_{2-x}$ and MoS_2
S. S. Jo, A. Singh, L. Yang, S. C. Tiwari, S. Hong, A. Krishnamoorthy, M. G. Sales, S. M. Oliver, J. Fox, R. L. Cavalero, D. W. Snyder, P. M. Vora, S. J. McDonnell, P. Vashishta, R. K. Kalia, A. Nakano, and R. Jaramillo
Nano Letters **20**, 8592-8599 (2020).

453. Simultaneous observation of carrier-specific redistribution and coherent lattice dynamics in 2H-$MoTe_2$ with femtosecond core-level spectroscopy
A. R. Attar, H.-T. Chang, A. Britz, X. Zhang, M.-F. Lin, A. Krishnamoorthy, T. Linker, D. Fritz, D. M. Neumark, R. K. Kalia, A. Nakano, P. Ajayan, P. Vashishta, U. Bergmann, and S. R. Leone
ACS Nano **14**, 15829-15840 (2020).

454. MISTIQS: an open-source software for performing quantum dynamics simulations on quantum computers
C. Powers, L. Bassman, T. M. Linker, K. Nomura, S. Gulania, R. K. Kalia, A. Nakano, and P. Vashishta
SoftwareX **14**, 100696: 1-6 (2021).

455. Mechanical behavior of ultralight nickel metamaterial
P. Rajak, A. Nakano, P. Vashishta and R. K. Kalia
Applied Physics Letters **118**, 081902:1-4 (2021).

456. Sulfurization of MoO_3 in chemical vapor deposition synthesis of MoS_2 enhanced by an H2S/H2 mixture
S. Hong, S. Tiwari, A. Krishnamoorthy, K. Nomura, C. Sheng, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta
Journal of Physical Chemistry Letters **12**, 1997-2003 (2021).

457. Lattice thermal transport in two-dimensional alloys and fractal heterostructures
A. Krishnamoorthy, N. Baradwaj, A. Nakano, R. K. Kalia, and P. Vashishta
Scientific Reports **11**, 1656:1-8 (2021).

458. EZFF: Python library for multi-objective parameterization and uncertainty quantification of interatomic forcefields for molecular dynamics
A. Krishnamoorthy, A. Mishra, D. kamal, S. Hong, K. Nomura, S. C. Tiwari, A. Nakano, R. K. Kalia, R. Ramprasad and P. Vashishta
SoftwareX **13**, 100663:1-9 (2021).

459. Carrier-specific dynamics in 2H-$MoTe_2$ observed by femtosecond soft X-ray absorption spectroscopy using an X-ray free-electron laser
A. Britz, A. R. Attar, X. Zhang, H.-T. Chang, C. Nyby, A. Krishnamoorthy, S. H. Park, S. Kwon, M. Kim, D. Nordlund, S. Sainio, T. F. Heinz, S. R. Leone, A. M. Lindenberg, A. Nakano, P. Ajayan, P. Vashishta, D. Fritz, M.-F. Lin, and U. Bergmann
Structural Dynamics **8**, 014501:1-10 (2021).

460. Domain-specific compilers for dynamic simulations of quantum materials on quantum computers
L. Bassman, S. Gulania, C. Powers, R. Li, T. Linker, K. Liu, T. K. S. Kumar, R. K. Kalia, A. Nakano, and P. Vashishta
Quantum Science and Technology **6**, 014007: 1-12 (2021).

461. Dielectric constant of liquid water determined with neural network quantum molecular dynamics
A. Krishnamoorthy, K. Nomura, N. Baradwaj, K. Shimamura, P. Rajak, A. Mishra, S. Fukushima, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Physical Review Letters **126**, 216403 (2021).

462. Unveiling oxidation mechanism of bulk ZrS_2
L. Yang, S. C. Tiwari1, S. S. Jo, S. Hong, A. Mishra, A. Krishnamoorthy, R. K. Kalia, A. Nakano, R. Jaramillo, and P. Vashishta
MRS Advances (2021) **6**:303–306.

463. PND: Physics-informed neural-network software for molecular dynamics applications
T. M. Razakh, B. Wang, S. Jackson, R. K. Kalia, A. Nakano, K. Nomura, and P. Vashishta
SoftwareX **15**, 100789: 1-5 (2021).

464. Autonomous reinforcement learning agent for chemical vapor deposition synthesis of quantum materials
P. Rajak, A. Krishnamoorthy, A. Mishra, R. K. Kalia, A. Nakano and P. Vashishta
npj Computational Materials **7**, 108: 1-9 (2021.

465. Autonomous reinforcement learning agent for stretchable kirigami design of 2D materials
P. Rajak, B. Wang, K. Nomura, Y. Luo, A. Nakano, R. K. Kalia and P. Vashishta
npj Computational Materials **7**, 102: 1-8 (2021).

466. Neural network quantum molecular dynamics, intermediate range order in GeSe2, and neutron scattering experiments
P. Rajak, N. Baradwaj, K. Nomura, A. Krishnamoorthy, J. P. Rino, K. Shimamura, S. Fukushima, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
Journal of Physical Chemistry Letters **12**, 6020-6028 (2021).

467. Dielectric polymer property prediction using recurrent neural networks with optimizations
A. L. Nazarova, L. Yang, K. Liu, A. Mishra, R. K. Kalia, K. Nomura, A. Nakano, P. Vashishta, and P. Rajak
Journal of Chemical Information and Modeling **61**, 2175-2186 (2021).

INVITED TALKS

- Melting of a Two-Dimensional Electron Solid
  Annual Meeting of the American Physical Society, Phoenix, AZ, March 1981.
- Molecular Dynamics Study of 2D Melting: Long Range Potentials
  NATO Advanced Study Institute on Nonlinear Phenomena at Phase Transitions and Instabilities, Geilo, Norway, March 29-April 9, 1981.
- Melting and Nucleation of a Two-Dimensional Coulomb Solid
  International Conference on Physics of Intercalation Compounds, I.C.T.P. Trieste, Italy, July 6-10, 1981.
- Melting and Freezing in Two Dimensions: A Molecular Dynamics Study
  9th Midwest Solid State Theory Symposium, Argonne National Laboratory, Argonne, IL. Nov. 2-3, 1981.
- Electrons on Smooth and Corrugated Surfaces
  10th Midwest Solid State Theory Symposium, Michigan State University, East Lansing, MI, Oct. 8-9, 1982.
- Microscopic Structure of Electron Glass in Two Dimensions
  12th Midwest Solid State Theory Symposium, University of Minnesota, October 1984.
- Fractal Dimensions of Brown Trails and Isosets in Superionic and Molten Ag_2I
  Electrochemical Society Meeting, Las Vegas, NV, October 14-18, 1985.
- Monte Carlo and Molecular Dynamics Simulations of Condensed Matter Systems
  Workshop on the Electronic Structure of Defects, Argonne National Laboratory, Argonne, IL, June 2-13, 1986.
- Random Resistance Fluctuations in 1D MOSFETs
  Summer Institute in Theoretical Physics, Workshop on the Physics of Artificially Structured Materials, 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 Condensed Matter Theory, 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 Condensed Matter Theories, Taxco, Mexico, August 14-20, 1988.
- Quantum Molecular Dynamics Simulations
  CECAM Meeting on Computational Problems of Glasses and Networks, 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.
- 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
- Workshop on Solution-phase self-assembly: From periodic superlattices to functional hierarchical architectures
  University of Nebraska, September 22, 2016
- Plasticity and Fracture in Disordered Systems
  The Institute of Mathematical Sciences, Chennai, India, January 4-7, 2017
- Petascale Simulations of Structural Phase Transformations and Fracture
  International Conference on Microstructural Functionality at the Nanoscale, University of Duisburg, Germany, October 4-6, 2017.
- Co-Organizer, Symposium on "Materials Genome Towards Exascale", Spetses, Greece, June 10-15, 2018.
- Co-Organizer, 4 Focus Sessions on "Emerging Trends in Molecular Dynamics Simulations and Data Analytics", at the 2019 APS March Meeting, Boston, MA.
- Deep Learning of CVD Growth and Phase-Transition Pathways in Layered Materials
  International Conference on Electric Field Enhanced Processing of Advanced Materials II: Complexities and Opportunities, March 10-15, 2019, Tomar, Portugal.
- Deep Learning for Nanosystem
  Plenary Lecture at the 2019 CINT Annual Meeting, Santa Fe, NM, September 22-24, 2019.
- Co-Organizer, Focus Sessions on "Emerging Trends in Molecular Dynamics Simulations and Machine Learning", at the 2020 APS March Meeting.
- AI-driven modeling & cybermanufacturing of quantum material architectures
  Conference on "Artificial Intelligence in Multi-Fidelity, Multi-Scale, and Multi-Physics Simulation of Materials", Oak Ridge National Laboratory, August 2-4, 2021.
- Deep Learning in materials simulations
  Beyond Fingerprinting Seminar, Sandia National Laboratories, December 16, 2021
- AI-driven modeling and simulations of quantum materials
  Invited Talk, APS March meeting, Chicago, IL, March 14-18, 2022.

- Machine Learning Innovations in Materials Design
  Colloquium, Materials Science Department, University of California, Irvine, January 20, 2022