PRIYA VASHISHTA

Collaboratory for Advanced Computing and Simulations

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CURRENT POSITION: Director, Collaboratory for Advanced Computing and Simulations
University of Southern California
Professor of Chemical Engineering & Materials Science, Physics & Astronomy, and Computer Science

EDUCATION: Ph.D., Indian Institute of Technology, Kanpur, India, 1967

PERSONAL: Born August 24, 1944; Wife: Annie-Claude; US Citizen; Naturalization Date: May 1, 1995

PROFESSIONAL EXPERIENCE

2002 - Present Director, Collaboratory for Advanced Computing and Simulations (CACS), and Professor of Chemical Engineering & Materials Science, Physics and Astronomy, and Computer Science, University of Southern California
1990 - 2002 Founding Director, Concurrent Computing Laboratory for Materials Simulations (CCLMS), Louisiana State University, Baton Rouge
1990 - 2002 Cray Professor of Computational Sciences, Louisiana State University, Baton Rouge
1984 - 1990 Senior Scientist, Argonne National Laboratory
1979 - 1982 Director, Solid State Science Division, Argonne National Laboratory
1972 - 1979 Member of the Research Staff, Argonne National Laboratory
1971 - 1972 Assistant Professor, Western Michigan University
1970 - 1971 Assistant Professor, Northwestern University

CONCURRENT POSITIONS

1986 - 1987 Visiting Scientist, Cornell Theory Center and LASSP, Cornell University with Kenneth Wilson (*Nobel Prize, 1982*)
1983 Visiting Scientist, Institute for Theoretical Physics, UC-Santa Barbara
1982 - 1985 Adjunct Professor of Physics, Northwestern University
1976 - 1977 Visiting Professor, University of California at San Diego with Walter Kohn (*Nobel Prize, 1998*)
1976 Visiting Scientist, Bell Laboratories, Murray Hill, NJ
1972 Visiting Scientist, IBM Research Center, Yorktown Heights
1968 - 1970 Postdoctoral Research Associate, McMaster University, Hamilton, Ontario, Canada
1966 - 1968 Postdoctoral Fellow, St Andrews University, St. Andrews, Scotland

Awards and Honors

2013 The Best Paper Award, IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing
2010 University of Southern California Associates Award for Creativity in Research
2008 University of Southern California Engineering Faculty Senior Research Award
2002 Best Paper, IEEE Virtual Reality Conference
2001 The Best Technical Paper Award, IEEE/ACM Supercomputing Conference
1999 Fellow of the American Physical Society
1997 Sustained Excellence Performer Award in Ultra Dense, Ultra Fast Computing Components, DARPA

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1990 United Nations Development Program Fellowship Award for Research and Consultation in India
1989 Japan Society for the Promotion of Science Senior Fellowship Award for Research in Japan,
1985 Brazilian Science Research Council Fellowship Award for Research in Brazil
1985 Japan Society for the Promotion of Science Senior Fellowship Award for Research in Japan
1976 The University of Chicago Award for Distinguished Performance at Argonne National Laboratory

INVITED TALKS: 244; **TOTAL PUBLICATIONS: 386** papers; **11** edited books; **12** book chapters

VISION:

Computing technology will grow by a factor of more than a thousand in the next ten years. Our goal is to follow this computing revolution from petaflops (10^{15} flops) to exaflops (10^{18} flops). Using this unprecedented computing power, available for the first time in the history of science and engineering, it will be possible to carry out realistic simulations of complex systems and processes in the areas of nanostructured materials and processes, nanotechnology, and bioengineered systems. Coupled with immersive and interactive visualization this will offer unprecedented opportunity for research as well as modifying graduate and undergraduate education in physics and engineering.

COLLABORATORY FOR ADVANCED COMPUTING AND SIMULATIONS (CACS)

The CACS has two main objectives: i) multidisciplinary research involving computational grand challenges in materials and biological simulations, especially at the nano-bio interface; and ii) the development of undergraduate and graduate education in computational science and engineering.

RESEARCH INTERESTS

Multiscale simulations combining molecular dynamics with density functional theory for reactive processes and finite element for continuum behaviors on petascale supercomputers and as well as on future exascale computers. We are also designing multiresolution algorithms and visualization tools for 3D immersive and interactive virtual environments. Current simulation effort focuses on: 1) Residual stresses, nucleation and growth of cracks, stress corrosion, and delamination at metal/ceramic, semiconductor/ceramic interfaces; 2) sintering, structure, and fracture in nanophase ceramic composites; 3) shock propagation in ceramics and self-assembled monolayers; 4) nano-engineered energetic materials and munitions under extreme conditions; 5) pressure-induced structural transformations in semiconductor nanoparticles and nanorods; 6) nanoindentation and dynamic friction; 7) self organized monolayers (SAM) and hybrid physical and biological systems consisting of nanostructures linked with membranes, DNA and peptides; and 8) transfection of small interfering RNA across cell membranes.

EDUCATIONAL PROGRAMS

Dual-degree Program

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

Courses Taught

Basics of atomistic simulation of materials, molecular dynamics simulations of materials and processes; thermodynamics and statistical physics; solid state physics; freshmen academy.

OUTREACH

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

RESEARCH INFRASTRUCTURE

***Local parallel computing resources*:** We established a Collaboratory for Advanced Computing and Simulations (CACS) at USC in September 2002. The CACS has a 4,096-processor (3,072 Intel Xeon and 1,024 AMD Opteron) Linux cluster, with peak performance of 24 teraflops.

***Collaborative immersive and interactive visualization facilities*:** The CACS also has: 1) a 14'×8' tiled display driven by a 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 access to the IBM Blue Gene/L at Lawrence Livermore National Laboratory and IBM Blue Gene/P at Argonne National Labpratory via a DOE-INCITE grant (135 million core hours) for our SCiDAC project.

CONCURRENT COMPUTING LABORATORY FOR MATERIALS SIMULATION (*CCLMS*)

We established a *Concurrent Computing Laboratory for Materials Simulations (CCLMS)* in 1990 at LSU i) to conduct multidisciplinary research in computational materials sciences and ii) to develop interdisciplinary educational programs involving high performance computing and communications.

CCLMS Computational facilities: With $3 million in infrastructure enhancement grants from the State of Louisiana and federal agencies, the *CCLMS* is equipped with a number of parallel architectures—a Linux cluster connected by a hierarchical network fabric consisting of gigabit switches; a Digital Alpha cluster on Gigaswitches; and a 64-cell Intel iWarp systolic array architecture. *We brought the parallel clusters and Intel iWarp to USC in 2002.*

Visualization facilities: An immersive and interactive 3D virtual environment called *ImmersaDesk*; a multiprocessor SGI Onyx2 with an InfinityReality2 graphics pipeline; an SGI Octane MXE; and a number of SGI graphics workstations. *We also brought the ImmersaDesk to USC.*

Biological Computation And Visualization Center: In 2000 we received a five-year, $3.9 million competitive grant from the State of Louisiana to establish a Biological Computation and Visualization Center (BCVC). It involves faculty, postdocs, and graduate students from the biological, physical, and computer sciences, and engineering at Louisiana State University and A&M College in Baton Rouge and Louisiana State University Health Sciences Center in New Orleans. Multidisciplinary research activities within the *BCVC* focus on massively parallel simulations, data mining, and immersive and interactive visualization of biological applications. An important educational goal of the *BCVC* is to propel students into careers in emerging areas of biological and information technologies both in academic and industrial settings. In 2002, the BCVC also received a three-year, $5.9 million grant from the National Institute of Health.

ADMINISTRATIVE EXPERIENCE

From 1979-82, I was the Director of the Solid State Science Division at Argonne National Laboratory. The division consisted of 85 scientific and technical personnel, including 50 Ph.D.-level scientists. My job involved securing block funding from the Department of Energy and overseeing various research and instrument development programs. During my tenure, the division was also involved in the establishment of a DOE supported $50 million facility called the Intense Pulsed Neutron Source (IPNS). The IPNS, during its operation, was recognized as one of the best pulsed neutron research facilities in the world.

MULTIINSTITUTIONAL, MULTIDISCIPLINARY ACTIVITIES

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

NSF-PetaApps, "Petascale Hierarchical Simulations of Biopolymer Translocation through Silicon Nitride and Silica Nanopores and Nanofluidic Channels": We are spearheading (Kalia, Nakano, Vashishta—PI) a $2M project with UC Santa Barbara (H. Metiu), Utah (M. Hall) and Purdue (A. Grama) to perform hybrid quantum mechanical-atomistic-mesoscale simulations of ion transport and translocation of biopolymers such as DNA and RNA through nanometer scale pores and channels in silica and silicon nitride membranes.

NSF-EMT (Emerging Models and Technologies for Computation), "Petascale Simulations of DNA Dynamics and Self-Assembly": We are spearheading (Kalia, Nakano, Vashishta—PI) this EMT project with Purdue (A. Grama) to develop a predictive hierarchical petascale simulation framework to study DNAs through solid-state nanopores and shear-induced DNA self-assembly.

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

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

DOE-EFRC (Energy Frontier Research Center) "Emerging Materials for Solar Energy Conversion

and Solid State Lighting*":*** This $12M EFRC involves collaboration between University of Southern California, University of Illinois, University of Michigan and University of Virginia. Research at the Center is focused on emerging materials for solar energy and solid-state lighting and the invention of new solar cell and LED designs based on nanostructured and organic materials. Multimillion atom simulations of nanostructured materials will be carried out by Kalia, Nakano and Vashishta at USC.

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

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

CURRENT RESEARCH FUNDING

1. "Hierarchical petascale simulation framework for stress corrosion cracking"
   P. Vashishta, R. K. Kalia, A. Nakano, jointly with Harvard, Purdue, Cal State-Northridge, Los Alamos, and Lawrence Livermore
   Department of Energy, SCiDAC (Scientific Discovery through Advanced Computing) Program, CACS portion: $1,475,000 for 5 years
2. DTRA: Molecular Mechanisms of Spore Killing by Corrosive and Detonation Product Gases: Reactive Molecular Dynamics Coupled with Graph-Theoretic Methods
   DoD DTRA: $750,000 for 5 years
3. Supplemental for "Hierarchical petascale simulation framework for stress corrosion cracking"
   P. Vashishta (PI), R. K. Kalia, A. Nakano
   DOE, SciDAC (Scientific Discovery through Advanced Computing), $216,000 for 2 years
4. "Synthesis, characterization, and multiscale simulations of low-cost high density insensitive high performance energetic composite molecular systems"
   P. Vashishta, R. K. Kalia, A. Nakano, K Christe (USC); D. S. Stewart (UIUC); Y. Gupta (WSU)
   Office of Naval Research, $3,175,000 for 5-years
5. "Petascale hierarchical simulations of biopolymer translocation through silicon nitride and silica nanopores and nanofluidic channels"
   P. Vashishta, R. K. Kalia, A. Nakano, M. Hall, jointly with UC, Santa Barbara
   National Science Foundation, PetaApps Program, CACS portion: $1,575,000 for 5 years
6. "Probing complex dynamics of small interfering RNA (siRNA) transfection by petascale simulations"
   P. Vashishta, R. K. Kalia, A. Nakano (USC)
   National Science Foundation, Collaborative Research: CDI-Type II, $1,080,000 for 4 years
7. "Petascale simulations of DNA dynamics and self-assembly"
   P. Vashishta, R. K. Kalia, A. Nakano, jointly with Purdue University
   National Science Foundation, Emerging Models and Technologies for Computation (EMT) Program, CACS portion: $450,000 for 3 years

8. "Emerging materials for solar energy conversion and solid state lighting"
   P. D. Dapkus (PI), M. E. Thompson, P. Vashishta, R. K. Kalia, A, Nakano, et al.; J. C. Campbell (UVa); J. J. Coleman (UIUC); and S.R. Forrest (UM)
   Department of Energy, Energy Frontier Research Center, CACS portion: $12,000,000 for 5 years

9. "Cholesterol flip-flop dynamics and nanomechanical response of deformed biomembranes: experiments and petascale simulations"
   N. Malmstadt, R. K. Kalia, A. Nakano, P. Vashishta
   National Science Foundation, $450,000 for 3 years

10. "Computational science workshop for underrepresented groups"
    R. K. Kalia, A. Nakano, and P. Vashishta
    DoD High Performance Computing Modernization Program (HPCMP), $721,000 for 6 years

SERVICE AT USC

High Performance Computing and Communications (HPCC) at USC

1. Faculty Advisory Council on High Performance Computing and Communications Committee, Chair, 2004-present
2. Cyberinfrastructure Architecture Committee, 2004-2005

USC Wide Committees:

3. Provosts Committee on ISD Reorganization, 2005-2006
4. Joint USC Senate and Provost Committee on Research, 2005-2006
5. Provost Strategic Planning Committee, 2008-2009
6. Graduate School Committee on Fellowships, Prizes, and Awards, 2008-2010
5. Provost Strategic Planning Committee, 2009-2011
7. Applied Mathematics task force, 2009

School of Engineering:

8. Provost Committee for the Search of Dean of School of Engineering, 2005-2006
9. Engineering Faculty Council, 2004-2006
10. Committee for the Merger of Chemical Engineering and Materials Science, 2004-2005
11. Green Engineering Curriculum Committee, 2010-2013
12. APT Committee, 2010-2012
13. Transformative Faculty Hire Committee, Chair, 2010-2013

Mork Family Department of Chemical Engineering and Materials Science

14. Chemical Engineering Centennial Committee, 2005-2006
15. EFC appointed MFD Chair evaluation committee, 2009
16. Merit review Committee, 2008-2013
17. Ping Lecture committee, 2009
18. Spitzer Lecture committee, Chair, 2012
19. MFD Executive Committee, 2011-2013

Dornsife College of Letters, Arts and Sciences :

20. College Initiatives Advisory Committee, 2003-2004

21. Physics and Astronomy Executive Committee, 2005-2006

CONFERENCE ACTIVITIES [CONFERENCE CHAIRMAN/CO-CHAIRMAN]:

- 26th "Midwest Solid State Conference", Argonne National Laboratory, November 1978
- International Conference on "Fast Ion Transport in Solids", Lake Geneva, Wisconsin, May 1979
- International Conference on "Ordering in Two Dimensions", Lake Geneva, Wisconsin, May 1980
- 29th Midwest Solid State Conference on "Novel Materials and Techniques in Condensed Matter", September 1981
- 9th Midwest Solid State Theory Symposium on "Melting, Localization and Chaos", November 1981
- Workshop on "Phase Transitions and Gauge Theories," Argonne National Laboratory, July 19 - September 10, 1982
- "Rahman Festschrift", Argonne National Laboratory, November 12-13, 1984
- X Pan American Workshop on "Condensed Matter Theories," Argonne National Laboratory, July 21-26, 1986
- "Highlights in Condensed Matter Physics", International Center for Theoretical Physics, Trieste, Italy, August 1-3, 1989
- "Concurrent Computing in the 90's", Louisiana State University, August 17, 1990
- "Undergraduate and Graduate Education in Computational Sciences", Louisiana State University, April 29-30, 1991
- "Parallel Computing Adventure: An Enrichment Course for High School Teachers", Louisiana State University, August 3-7, 1992
- International Conference on "Concurrent Computing in the Physical Sciences", Louisiana State University, February 18-20, 1993
- International Conference on "Toward Teraflop Computing and New Grand Challenge Applications", Louisiana State University, February 10-12, 1994
- Symposium on "Grand Challenges in Computer Simulations" at the High Performance Computing '94 of the Society of Computer Simulation in La Jolla, CA, April 11-15, 1994.
- International Conference on "High Performance Computing Technologies and Scientific Applications", Louisiana State University, February 23-25, 1995
- "High Performance Computing Symposium" at The Simulation Multiconference, The Society of Computer Simulation, Phoenix, AZ, April 9-13, 1995
- "XIX International Workshop on "Condensed Matter Theories", Caracas, Venezuela, June 12-17, 1995
- "Computational Physics Workshop for Undergraduate Students", Louisiana State University, July 17-28, 1995
- "Materials Theory, Simulation, and Parallel Algorithms", A five day Symposium at the Annual Meeting of the Materials Research Society, Boston, MA, November 27-December 1, 1995
- International Conference on " Experimental and Simulation Challenges in Nanostructured Materials", Louisiana State University, February 15-17, 1996
- International Materials Research Congress Symposium on "Computational Materials Science: Theory and Simulation of Nanostructured Materials", Cancun, Mexico, September 1-6, 1996

- International Conference on "Multiscale Phenomena in Science and Engineering", Louisiana State University, February 7-9, 1997
- International Conference on "Computer-Aided Design of High-Temperature Materials", Santa Fe, NM, July 30-August 2, 1997
- International Materials Research Congress Symposium on "Theory and Computer Simulation of Materials: Electronic Structure and Mechanical Behavior", Cancun, Mexico, September 1-5, 1997
- International Conference on "Materials and Microsystems for Extreme Environments: Experimental and Computational Challenges", Louisiana State University, February 19-21, 1998
- International Conference on "Thermo-Mechanical and Electrical Properties of High-Temperature Materials", Maui, HI, January 4-9, 1999
- Workshop on "Parallel Algorithms, Computational Efficiency and Multiscale Materials Simulations", April 2-3, 1999, New Orleans, LA
- International Materials Research Congress Symposium on "Theory and Computer Simulation of Materials - Matching of Length Scales in Materials Science: Electronic, Atomic and Continuum Properties of Materials", Cancun, Mexico, August 29-September 2, 1999
- International Conference on "Materials Design: Experimental and Computational Challenges", Louisiana State University, March 2-4, 2000
- International Conference on "Multiscale Materials Phenomena in Harsh Environments", Limassol, Cyprus, June 19-24, 2000
- International Conference on "Multiscale Simulation, Theoretical, and Experimental Approaches to Deformation, Friction, Fatigue, and Fracture", Louisiana State University, Baton Rouge, February 22-24, 2001
- "Computational Science Workshop for Underrepresented Groups", Louisiana State University, January 4-10, 2002
- Mardi Gras 2002 Conference on "Nanotechnology at the Interface of Information Technology" Louisiana State University, February 7-9, 2002
- "35th Year Anniversary of the Materials Science Department and the Inauguration of the Collaboratory for Advance Computing and Simulations at USC", University of Southern California, November 8, 2002
- "Computational Science Workshop for Underrepresented Groups", Louisiana State University, January 5-11, 2003
- Mardi Gras 2003 Conference on "Grid Computing and Simulation at the Nano-Bio Interface", Louisiana State University, February 27-March 1, 2003
- "Computational Science Workshop for Underrepresented Groups", University of Southern California, January 5-10, 2004
- "*Computational and Experimental Challenges in Physical, Chemical and Biological Systems*", August 20-21, 2004, Univ. of Southern California, Los Angeles, CA.
- "*Computational Science Workshop for Underrepresented Groups*",January 5-11, 2005, University of Southern California, Los Angeles, CA.
- "*Computational Science Workshop for Underrepresented Groups*", January 5-11, 2006, University of Southern California, Los Angeles, CA.
- "*Computational Science Workshop for Underrepresented Groups*", January 3-10, 2007, University of Southern California, Los Angeles, CA.
- "*Computational Science Workshop for Underrepresented Groups*" May 18-25, 2008, University of Southern California, Los Angeles, CA.

- Symposium on "Scientific Discovery through Advanced Computing and Experiments", International Conference on Computing & Experimental Engineering and Sciences, April 8-13, 2009, Phuket, Thailand
- "*Computational Science Workshop for Underrepresented Groups*"
  June 21-29, 2009, University of Southern California, Los Angeles, CA.
- USC-DOE conference on "*Emerging Trends in Materials Simulations and Experiments*"
  March 24-26, 2010, Terranea Resort in Greater Los Angeles, CA.
- USC-DOE conference on "*Materials for Energy Applications - Experiment, Modeling and Simulations*"
  March 30-April 1, 2011, Terranea Resort in Greater Los Angeles, CA.
- USC-DOE conference on "Materials Genome: Simulations, Synthesis, Characterization and Manufacturing"
  April 4-6, 2012, Terranea Resort in Greater Los Angeles, CA.
- Symposium on "DNA Directed Self-assembly of Nanoparticles into Meta Materials for Energy and Other Applications"
  European Materials Research Society Spring Meeting, May 14-18, 2012, Strasbourg, France
- Western Regional Workshop on the Materials Genome Initiative
  April 7, 2014, Los Angeles, CA.

BOOKS, BOOK CHAPTERS, AND ARTICLES:

BOOKS:

1. Fast Ion Transport in Solids, (1979), Elsevier North-Holland, New York,
   Editors: P. Vashishta, J. N. Mundy and G. K. Shenoy
2. Novel Materials and Techniques in Condensed Matter, (1982), Elsevier North-Holland, New York
   Editors: G. W. Crabtree and P. Vashishta
3. Melting, Localization and Chaos, (1982), Elsevier North-Holland, New York
   Editors: R. K. Kalia and P. Vashishta
4. Condensed Matter Theories, Vol. 2, (1987), Plenum Press, New York
   Editors: P. Vashishta, R. K. Kalia, and R. Bishop
5. Correlations in Electronic and Atomic Fluids, (1990), World Scientific, Singapore
   Editors: P. Jena, R. K. Kalia, M. P. Tosi, and P. Vashishta
6. High Performance Computing and its Applications in the Physical Sciences, (1993), World Scientific
   Editors: D. A. Browne, J. Callaway, J. P. Draayer, R. W. Haymaker, R. K. Kalia, J. E. Tohline, and, P. Vashishta
7. Teraflop Computing and New Grand Challenge Applications, (1995), Nova Publishing
   Editors: R. K. Kalia and P. Vashishta
8. Condensed Matter Theories, Vol 11, (1995), Nova Publishing, New York
   Editors: E. V. Ludena, P. Vashishta, and R. F. Bishop
9. Materials Theory, Simulations, and Parallel Algorithms, (1996), Materials Research Society Pittsburgh, Pennsylvania
   Editors: E. Kaxiras, J. Joannopoulos, P. Vashishta, and R. K. Kalia
10. Computer-Aided Design of High-Temperature Materials, (1998), Oxford Univ. Press, Oxford
    Editors: A. Pechenik, R. K. Kalia, and P. Vashishta
11. Applying Molecular and Materials Modeling, (2002), Springer
    Editors: P. R. Westmoreland, P. A. Kollman, A.M. Chaka, P. T. Cummings, K. Morokuma, M. Neurock, E. B. Stechel, and P. Vashishta

BOOK CHAPTERS:

1. *Melting and Freezing in Two Dimensions: A Molecular Dynamics Study*, Priya Vashishta and Rajiv K. Kalia, in Melting, Localization and Chaos, Editors: R. K. Kalia and P. Vashishta, Elsevier North-Holland, New York (1982), p. 43.
2. *General Density Functional Theory*, Walter Kohn and Priya Vashishta, in Inhomogeneous Electron Gas, Editors: N. H. March (Oxford, England) and S. Lunqvist (Chalmers, Sweden), Plenum, New York (1983), p. 79.
3. *Molecular Dynamics Study of Superionic Conductors*, Aneesur Rahman and Priya Vashishta, in Physics of Superionic Conductors, Editors: J. W. Perram (Odense, Denmark), Plenum, New York (1983), p. 93.
4. *Theory of Electron-Hole Liquid*, Priya Vashishta, Rajiv K. Kalia and Kundan S. Singwi, in Electron-Hole Droplets in Semiconductors, Editors: C. D. Jeffries (Berkeley, USA), L. V. Keldysh (Moscow, USSR) and North-Holland, Amsterdam (1983), p. 1.

BOOKS, BOOK CHAPTERS, AND ARTICLES:

5. *New Forms of Molecular Dynamics and Superionic Conductors*
John R. Ray, Aneesur Rahman, and P. Vashishta, Superionic Solids and Solid Electrolytes--Recent Trends, Editors: A. Laskar and S. Chandra,. Academic Press, New York (1987), p.

6. *Molecular Dynamics Methods and Large-scale Simulations of Amorphous Materials*
P. Vashishta, R. K. Kalia, A. Nakano, W. Li, and I. Ebbsjö, in Amorphous Insulators and Semiconductors, Eds: M. F. Thorpe and M. I. Mitkova, Kluwer, Dordrooht (1996) p. 151-213.

7. *Structure and Mechanical Failure in Nanophase Silicon Nitride: Large-scale Molecular-Dynamics Simulations on Parallel Computers*
A. Omeltchenko, A. Nakano, K. Tsuruta, R. K. Kalia, and P. Vashishta, in Advances in Metal and Semiconductor Clusters Vol. IV: Cluster Materials, Editor: M. Duncan, JAI Press, Stamford, CN (1998), pp. 263-298.

8. *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
in *Annual Review of Materials Research*, *Vol. 32*, edited by D. R. Clarke and M. Rühle (Annual Reviews, Palo Alto, CA, 2002) pp. 377-400

9. *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

10. *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) pp. 875-928

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

12. *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

BOOKS, BOOK CHAPTERS, AND ARTICLES:

ARTICLES:

1. Effect of Impurities on Magnetization of Ferromagnets at Low Temperatures
   P. Vashishta and J. Mahanty, Proc. Phys. Soc. **84**, 309 (1964)

2. Interaction of Impurities in a Ferromagnet at Low Temperatures
   P. Vashishta and J. Mahanty, Proc. Phys. Soc. **85**, 1215 (1965)

3. Spin Waves in Body-Centered Cubic and Face Centered Cubic Ferromagnets with a Substituted Impurity
   P. Vashishta, Proc. Phys. Soc. **91**, 372 (1967)

4. Nearest Neighbor Exchange Interaction of Manganese in Dilute Iron-Manganese Alloy
   P. Vashishta, Phys. Letters **26**A, 191 (1968)

5. Magnetization of an Antiferromagnetically Coupled Impurity in a Heisenberg Ferromagnet in R.P.A.
   P. Vashishta, Solid State Commun. **7**, 1253 (1969)

6. Mössbauer Recoiless Fraction of Solid Krypton
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INVITED TALKS AT CONFERENCES:

1. Ground State Energy Calculation of the Electron-Hole Liquid in Semiconductors
   P. Vashishta, P. Bhattacharyya and K. S. Singwi, Perspectives in Calculation of the Many-Electron Interactions in Solids, Taormina, Italy, Sept. 17-21 (1973)
2. Ground State Properties of the Electron-Hole Liquid in Ge and Si
   P. Vashishta, Symposium of the Division of Solid State Physics, American Physical Society Meeting, Philadelphia, Pennsylvania, March 25-28 (1974)
3. Surface Properties of Electron-Hole Drops in Germanium
   P. Vashishta, Oji Seminar on Physics of Highly excited States in Solids, Tomakomai City, Hokkaido, Japan, Sept. 10-13 (1975)
4. Surface Properties of Electron-Hole Liquid in Germanium
   P. Vashishta, Midwest Theoretical Solid State Physics Symposium, Purdue University, West Lafayette, Indiana, Nov. 10-11 (1975)
5. Electron-Hole Drops in Semiconductors
   P. Vashishta, NATO Advanced Institute on Strongly Coupled Plasmas, Universite d'Orleans, Orleans-la-Source, France, July 6-23, (1977)
6. Electron-Phonon Interaction in Transition Metals
   P. Vashishta, CECAM Workshop on Electron-Phonon Interactions, Orsay, France, July 18 - Sept. 2, (1977)
7. Electron-Phonon Interaction in Transition Metals and Alloys
   P. Vashishta, Midwest Theoretical Solid State Physics Symposium, Argonne National Laboratory, Argonne, Illinois, Oct. 17-18 (1977)
8. Nature of Ionic Motion in AgI and CuI
   P. Vashishta, International Conference on Fast Ion Transport in Solids, Lake Geneva, Wisconsin, May 21-25 (1979)
9. Molecular Dynamics Studies of Superionic Conductors
   P. Vashishta, NATO Advanced Study Institute on Physics of Superionic Conductors, Odense, Denmark, Aug. 11-23 (1980)
10. Nature of Ionic Motion in Superionic Conductors
    P. Vashishta, International Meeting on Solid Electrolytes-Solids State Ionics and Galvanic Cells,Tokyo, Japan, Sept. 15-19 (1980)
11. Nature of Order-Disorder Transition in Superionic Conductors
    P. Vashishta, Symposium of the Division of Condensed Matter Physics, American Physical Society Meeting, Phoenix, Arizona, March 16-20 (1981)
12. Molecular Dynamics Study of 2D Melting
    P. Vashishta, NATO Advance Study Institute on Nonlinear Phenomena at Phase Transitions and Instabilities, Geilo, Norway, March 29-April 9 (1981)
13. Melting and Nucleation of a Two-Dimensional Coulomb Solid
    R. K. Kalia and P. Vashishta, International Conference on Physics of Intercalation Compounds, I.C.T.P. Trieste, Italy, July 6-10 (1981)
14. Melting and Freezing in Two Dimensions
    P. Vashishta, 9th Midwest Solid State Theory Symposium on Melting, Localization and Chaos, Argonne National Laboratory, Argonne, Illinois, Nov. 2-3 (1981)
15. Strategic Planning for Solid State Science Research and Free Electron Laser Facility
    P. Vashishta, 83rd Meeting of Argonne University Association Board of Trustees,

INVITED TALKS AT CONFERENCES:

Carnegie-Mellon University, July 12-13 (1982)

16. Melting, Freezing and Order-disorder Transition in 2-Dimensions
P. Vashishta, VIth Pan American Workshop on Condensed Matter Theories, Washington University, St. Louis, MO, Sept. 20-Oct. 1 (1982)

17. Mass and Charge Transport in Solid Electrodes and Electrolytes
P. Vashishta, American Institute of Chemical Engineers Annual Meeting, Los Angeles, California, Nov. 14-18 (1982)

18. Melting on Corrugated Surfaces
P. Vashishta, NATO Advanced Study Institute on Multicritical Phenomena, Geilo, Norway, April 10-21 (1983)

19. Melting and Freezing Transitions on Corrugated Surfaces
P. Vashishta, Third International Conference on Recent Progress in Many-Body Theories, Altenberg, West-Germany, August 29-September 3 (1983)

20. Anisotropic Coulomb Liquids and Structural Phase Transitions
P. Vashishta, Eighth Workshop on Condensed Matter Theories, Granada, Spain, Sept. 17-28, 1984

21. Ionic Transport and Structural Phase Transitions in Superionic Conductors
P. Vashishta, American chemical Society Symposium on "Transport Phenomena in Solids and Related Systems", Miami, April 29 - May 3, 1985

22. Glasses in Two dimensions
P. Vashishta, Annual Brazilian Physical Society Meeting, Sao Laurenco, M. G., Brazil, May 29-June 1, 1985

23. Fractal Dimensionalities of Brownian Trajectories and Brown Isosets in Two Dimensions
P. Vashishta, Workshop on Many-Body Theories, San Francisco, CA, August 5-10, 1985

24. Structure and Dynamics of Superionic Conductors
P. Vashishta, International Conference on Many-Body Theories, San Francisco, CA, August 12-17, 1985

25. Use of Computer Simulation Techniques to Study Atomic Migration in Solids
P. Vashishta, International Conf. on Solid State Ionics, Lake Tahoe, CA, August 14-24, 1985

26. Electron Glass in Two Dimensions
P. Vashishta, Annual Meeting of the Japanese Physical Society, Chiba, Japan, October 1-4, 1985

27. Structure and Dynamics of Ions in Superionic Conductors
P. Vashishta, Conference on "Strongly Interacting Condensed Matter Systems," Hakone, Japan, October 11-15, 1985

28. Molecular Dynamics Study of Low-Lying States in Glasses
P. Vashishta, Annual Meeting of the American Physical Society, Las Vegas, NV, March 31-April 4, 1986

29. Simulation of Classical and Quantum Systems
P. Vashishta, Conference on "Statistical Physics and Phase Transformations," University of Sao Paulo, Sao Carlos, Brazil, January 5-9, 1987

30. Rings and Medium Range Order in Glasses
P. Vashishta, Workshop on "Computer Simulation Studies in Condensed Matter Physics" University of Georgia, Athens, Georgia, February 8-19, 1988

INVITED TALKS AT CONFERENCES:

31. Present and Future Applications of Molecular Dynamics
    P. Vashishta, Symposium in honor of Anees Rahman, Minnesota Supercomputer Institute, University of Minnesota, Minneapolis, Minnesota, March 30-31, 1988
32. Medium Range Order in Glasses
    P. Vashishta, XII International Workshop on Condensed Matter Theories, Taxco, Mexico, August 14-20, 1988
33. Intermediate Range Order in Chalcogenide Glasses
    P. Vashishta, CECAM Planning Workshop on Computational Problems of Glasses and Networks, Amersfoort, The Netherlands, September 10-14, 1988
34. Molecular Dynamics Simulation of Mass and Charge Transport in Superionic Conductors and Structural Correlations in Chalcogenide Glasses
    P. Vashishta, Materials Society Annual Meeting, Boston, MA, Nov. 28 - Dec. 3, 1988
35. Computer Simulation of Classical and Quantum systems Using Supercomputers
    P. Vashishta, Summer School on "Condensed Matter Physics", Australian National University, Canberra, Australia, January 9-27, 1989
36. Structural Correlations and Phonon Density of States in $GeSe_2$ -- A Molecular Dynamics Study of Molten and Amorphous States
    P. Vashishta, Workshop on "Molecular Dynamics Simulations", Laguna Beach, CA, March 9-11, 1989
37. Phonon Density-of-States, Isotope Effect, and Superconductivity in $Ba_xK_{1-x}BiO_3$
    P. Vashishta, "Many Body Encounter in Minnesota", Theoretical Physics Institute, University of Minnesota, Minneapolis, MN, May 12-14, 1989
38. Molecular Dynamics Study of the Structure and Dynamics of Network Glasses
    P. Vashishta, "Special Topics in Molecular Sieve Research: Synthesis -Structure- Simulation" Argonne National Laboratory, Illinois, June 14-15, 1989
39. Nature of Phonons and Isotope Effect in $Ba_xK_{1-x}BiO_3$
    P. Vashishta, "Highlights in Condensed Matter Theory", International Center for Theoretical Physics, Trieste, Italy, August 1-3, 1989
40. Vibrational Density-of-States, Isotope Effect, and Superconductivity in $Ba_xK_{1-x}BiO_3$ Cubic Oxides
    P. Vashishta, "Recent Progress in Condensed Matter Theories", Campos do Jordao, Brazil, August 7-11, 1989
41. Nature of Phonons,Isotope Effect, and Superconductivity in $Ba_xK_{1-x}BiO_3$
    P. Vashishta, Yamada Conference on "Strongly Coupled Plasmas", Lake Yamanaka, Japan, August 29 - September 1, 1989
42. Molecular dynamics Study of the Structure and Dynamics of Network Glasses
    P. Vashishta, 7th International Conference on "Solid State Ionics", Hakone, Japan, November 5-11, 1989
43. Molecular Dynamics Simulation of Chalcogenide Glasses
    P. Vashishta, Annual American Crystallographic Association Meeting, New Orleans, April 8-13, 1990
44. Intermediate Range Order in Glasses
    P. Vashishta, Workshop on “Many Body Encounter-90”, Clemson University, Clemson, South Carolina, May 4-6, 1990

INVITED TALKS AT CONFERENCES:

45. Molecular Dynamics Simulations of Molten and Glassy SiO_2, GeO_2, $SiSe_2$, and $GeSe_2$
P. Vashishta, International Symposium on "Molten Salts", Electrochemical Society Meeting, Montreal, May 7-11, 1990

46. Intermediate Range Order in Glasses
P. Vashishta, International Workshop on "Condensed Matter Theories", Elba, Italy, June 18-23, 1990

47. Role of Coulomb Interactions and Three-Body Forces in Network Glasses
P. Vashishta, CECAM Workshop on "Network Glasses", Orsay, France, July 2-13, 1990

48. Molecular Dynamics Study of Superionic Conductors and Network Glasses
P. Vashishta, International Conference on "Computer Applications to Material Science and Engineering", Tokyo, Japan, August 28-31, 1990

49. Computer Simulation of Glass Structures
P. Vashishta, Asian Conference on "Solid State Ionics", Beijing, China, October 29 - November 1, 1990

50. Ionic Transport in Network Glasses - A Molecular Dynamics Study
P. Vashishta, Symposium on "Solid State Ionics", Materials Research Society, Boston, November 26 - December 1, 1990

51. Nature of Phonons,Isotope Effect, and Superconductivity in $Ba_xK_{1-x}BiO_3$
P. Vashishta, Symposium on "Manifestations of the Electron-Phonon Interaction in Copper Oxides and Related Superconductors", Oaxtepec, Mexico, December 10-14, 1990

52. Crystalline Fragments in Glasses
P. Vashishta, International Symposium on "Frontiers of the Liquid and Amorphous State", Argonne National Laboratory, Illinois, August 12-15, 1991

53. Oxygen Isotope Effect in Superconducting $Ba_xK_{1-x}BiO_3$
P. Vashishta, XV International Workshop on "Condensed Matter Theories", Mar del Plata, Argentina, July 1-6, 1991

54. Computer Simulation of Network Glasses and Molecular Dynamics Algorithm on SIMD and MIMD Machines
P. Vashishta, Symposium on "Large-Scale Computations Applied to Many-Body Problems", Minnesota Supercomputer Institute, August 26-31, 1991

55. Parallel Algorithms for Molecular Dynamics Simulations on Distributed Memory MIMD Machines
P. Vashishta, Intel University Partner "Technology Focus Workshop", Timberline Lodge, Oregon, April 5-7, 1992

56. Microclusters Embedded in Zeolites: Atomistic Simulations on Parallel Architectures
P. Vashishta, "Domain-specific Methods for Massively Parallel Computational Science" Los Angeles, CA, May 14-15, 1992

57. Grand Challenges in Computer Simulation of Materials, Synthesis, and Processing
P. Vashishta, "Critical Technologies Research: Opportunities for DOE, Lawrence Berkeley Laboratory, Berkeley, CA, May 27-29, 1992

58. Molecular Dynamics Simulation of Network Glasses and MD Algorithm on Parallel (SIMD and MIMD) Architectures

INVITED TALKS AT CONFERENCES:

P. Vashishta, XVI Workshop on "Condensed Matter Theories", Puerto Rico, June 1-5, 1992

59. Structural and dynamical Correlations in Glasses
P. Vashishta, International Conference on the "Strongly Coupled Plasmas", Rochester University, August 17-21, 1992

60. Molecular Dynamics Simulations of Strongly Covalent Systems with Coulomb Interactions
P. Vashishta, International Meeting on "Computational Physics for Condensed Matter Phenomena", Tokyo, Japan, September 19-21, 1992

61. Molecular Dynamics Simulation of Network Glasses and MD Algorithm on Parallel (SIMD and MIMD) Architectures
P. Vashishta, The Second International Conference on "Computer Applications to Materials and
Molecular Science and Engineering", Yokohama, Japan, September 22-25, 1992

62. Covalent Glasses at Large Positive and Negative Pressures - A Molecular Dynamics Study
P. Vashishta, "New Developments of Computer Based Design of Functional Materials", Government Industrial Research Institute, Ministry of International Trade and Industry, Osaka, Japan, September 29-30, 1992

63. Classical and Quantum Simulations of Very large Systems on Parallel Computers
P. Vashishta, Invited Talk at the Annual Meeting of Materials Research Society, Boston, November 30-December 5, 1992

64. Structure and Dynamics of Network Glasses and Crystals at Large Positive and Negative Pressures
- A Molecular Dynamics Study
P. Vashishta, Invited Talk at the Annual Meeting of Materials Research Society, Boston, November 30-December 5, 1992

65. Molecular Dynamics Simulations of Covalent Glasses
P. Vashishta, Invited Talk at the American Physical Society Meeting, Oak Ridge, Tennessee, November 12-14, 1992

66. Covalent Glasses at Large Positive and Negative Pressures - A Molecular Dynamics Study
P. Vashishta, Invited Talk at the American Society for Materials, The Materials Society, Denver, Colorado, February 21-25, 1993

67. Structure and Dynamics of SiO_2 Glass at Large Positive and Negative Pressures
P. Vashishta, Invited Talk at the American Chemical Society, Denver, Colorado, March 28-April 2, 1993

68. Molecular Dynamics of Silica Under Very Large Positive and Negative Pressures on Parallel Computers
P. Vashishta, Invited Talk at the Simulation Multi Conference on High Performance Computing,
Washington DC, March 29 - April 1, 1993

69. Molecular Dynamics Simulations of Classical and Quantum Systems on Parallel Computers
P. Vashishta, Computational Approaches for Novel Condensed Matter Systems, Gordon Godfrey Workshop, University of New South Wales, Sydney, Australia, July 12-17, 1993

70. Quantum Molecular Dynamics Simulations of Solid C_{60} - the Effects of Orientational Disorder

INVITED TALKS AT CONFERENCES:

and Pressure
P. Vashishta, Symposium in Honor of John Quinn's 60th Birthday, Brown University, Rhode Island, September 3, 1993

71. Molecular Dynamics and Quantum Molecular Dynamics Simulations on Parallel Architectures
P. Vashishta, 2nd International Association for Mathematics and Computer Simulation Conference on Computational Physics, St. Louis, MO., October 6-9, 1993

72. Molecular Dynamics Simulations of Structure and Dynamics of Silica at Large Positive and Negative Pressures
P. Vashishta, The Minerals Metals Materials Society Meeting, Pittsburgh, PA., Oct. 17-21, 1993

73. Materials Simulations on Parallel Architectures
P. Vashishta, Future Directions of Quantum Many Body Theory, Texas A&M University, College Station, Texas, January 14-16, 1994

74. Computer Simulation of Porous Glasses on Parallel Architectures
P. Vashishta, High Performance Computing Symposium, The Society for Computer Simulation, San Diego,CA., April 11-14, 1994

75. Vibrational Spectra of Solid C_{60} and Graphitic Tubules - A Tight Binding Molecular Dynamics Study on Parallel Computers
P. Vashishta, Electrochemical Society Meeting, San Francisco, California, May 23-27, 1994

76. Multimillion Particle Molecular Dynamics Simulation of SiO_2 and Si_3N_4 on Parallel Computers
P. Vashishta, CECAM Workshop on Computer Simulation of the Growth of Semiconducting Materials, Lyon, France, May 30-June 2, 1994

77. Classical and Quantum Molecular Dynamics Simulations on Parallel Computers
P. Vashishta, VIII International Workshop on Condensed Matter Theories, Valencia, Spain, June 6-10, 1994

78. Molecular Dynamics Simulations of Silica at Large Positive and Negative Pressures on Parallel Computers
P. Vashishta, 12th Symposium on Thermophysical Properties, Boulder, CO., June 19-24, 1994

79. Computer Simulation of Materials on Parallel Architectures - Glasses, Solid C_{60}, and Graphitic Tubules
P. Vashishta, Oji International Seminar on Elementary Processes in Dense Plasmas, Tomakomai, Japan, June 27-July 1, 1994

80. Molecular Dynamics Simulations of Covalent Amorphous Insulators on Parallel Computers
P. Vashishta, Symposium on Amorphous Insulators, Pingree Park, CO., August 7-11, 1994

81. Molecular Dynamics Simulation of High Temperature Ceramics
P. Vashishta, Workshop on Large Scale Simulations in Chemistry and Materials Science, Dayton, Ohio, September 12-13, 1994

82. Large Scale Simulation of Silica on Parallel Computers
Quartz Workshop, Naval Research Laboratory, Washington, DC, Sept. 19-20, 1994

83. Molecular Dynamics Simulations of Glasses on Parallel Computers
P. Vashishta, 1995 Simulation Multiconference, The Society of Computer Simulation, Phoenix, AZ, April 9-13, 1995

84. Million Atom Simulations of Materials on Parallel Computers - Silica, Silicon Nitride, and

INVITED TALKS AT CONFERENCES:

Ceramic Thin Films
P. Vashishta, American Ceramic Society Meeting, Cincinnati, Ohio, May 1-3, 1995

85. Studies of Nanoclusters and Amorphous Materials by Parallel Molecular Dynamics Simulations
P. Vashishta, Annual Meeting of the American Ceramic Society, Cincinnati, Ohio, May 1-3, 1995

86. Massively Parallel Computing for Materials Modeling
P. Vashishta, Fifth Conference on Computational Research on Materials, University of West Virginia, WV, May 3-5, 1995

87. Crack Propagation and Fracture in Ceramic Films -- Million Atom Molecular Dynamics Simulations on Parallel Computers
P. Vashishta, Annual Meeting of the European-Materials Research Society Meeting, Strasbourg, France, May 22-26, 1995

88. Large Scale Simulation of Amorphous Materials
P. Vashishta, XIX International Workshop on Condensed Matter Theories, Caracas, Venezuela, June 12-17, 1995

89. Simulation of Crack Propagation and Fracture in Silica and Silicon Nitride Films on Parallel Computers
P. Vashishta, Amorphous and Crystalline Insulating Thin Films III Symposium at the Annual Meeting of Solid State Devices and Materials, Osaka, Japan, August 21-24, 1995

90. Crack Propagation and Fracture Glasses and Ceramics - Million Atom Molecular Dynamics Simulations on Parallel Computers
P. Vashishta, Recent Progress in Computational Materials Science Symposium at the IVth International Conference on Advanced Materials, Cancun, Mexico, Sept. 4-8, 1995

91. Million Atom Simulations of Real Materials on Parallel Computers
P. Vashishta, SURA/EPSCoR Workshop on Computational Materials, University of Kentucky, Lexington, October 9, 1995

92. Multimillion Particle Simulations of Real Materials on Parallel Computers
P. Vashishta, Materials Modeling'95, Naval Research Laboratory, Washington, DC, October 17-18, 1995

93. Molecular Dynamics Simulations of Glasses and Ceramic Materials Using Parallel Computers
P. Vashishta, Takahashi Symposium, Solid State Ionics-10, Singapore, December 3-8, 1995

94. Amorphous and Liquid Carbon, and Dynamic fracture - Molecular Dynamics Simulations on Parallel Computers
P. Vashishta, High Performance Computing Workshop in Computational Chemistry and Materials Science, Maui High Performance Computing Center, Maui, December 21-22, 1995

95. Million Atom Simulations of Ceramic Materials on Parallel Computers - Crack Propagation, Fracture, and Sintering in Silicon Nitride
P. Vashishta, American Ceramic Society, Annual Meeting, Indianapolis, April 14-17, 1996

96. Molecular Dynamics Method and Large Scale Simulation of Amorphous Materials
P. Vashishta, NATO Advanced Study Institute, Amorphous Insulators & Semiconductors, Sozopol, Black Sea Coast, Bulgaria, May 26 - June 8, 1996

97 Million Atom Molecular Dynamics Simulation on Parallel Computers

INVITED TALKS AT CONFERENCES:

P. Vashishta, "Theory Workshop", Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois, June 24-27, 1996

98. Amorphization and Fracture in Silicon Diselenide Nanowires - A Molecular dynamics study
P. Vashishta, International Materials Research Congress, September 1-6, 1996, Cancun, Mexico

99. Large-Scale Simulation of Crack Propagation and Fracture on Parallel Computers
P. Vashishta, Parallel Computing Conference, Minnesota Supercomputing Institute, Minneapolis, MN, October 3-4, 96.

100. Million Atom Simulations of Crack Propagation, Fracture, Sintering, and Densification of Ceramic Materials on Parallel Computers
P. Vashishta, Tsukuba Symposium on "Computer Simulations for Inorganic and Organic Materials and Biological Systems", Tsukuba, Japan, February 20, 1997

101. Million Atom Simulations of Crack Propagation, Fracture, Sintering, and Densification of Ceramic Materials on Parallel Computers
P. Vashishta, "International Symposium on Novel Materials", Puri, India, March 3-7, 1997.

102. Large Scale Computer Simulations of Glasses
P. Vashishta, Symposium on "Intermediate Range Order in Glasses", American Crystallographic Society of America, St. Louis, Mo, July 21-25, 1997

103. Molecular Dynamics Simulations of Si/Si3N4 Interface and Si/Si/Si3N4 Mesa on Parallel Computers
P. Vashishta, "The Second NASA Workshop on Semiconductor Device Modeling", NASA-Ames,
CA, August 7-8, 1997

104. Molecular Dynamics Simulations of Si/Si3N4 Interface and Si/Si/Si3N4 Mesa on Parallel Computers
P. Vashishta, Symposium on "Theory and Computer Simulation of Materials - Electronic, Structural, and Mechanical Properties", Mexican Materials Research Society, Cancun, Mexico, September 1-4, 1997

105. Multimillion Atom Simulations of Sintering, Crack Propagation, and Fracture on Parallel Computers
P. Vashishta, "Noncrystalline Materials", Ohio State University, Columbus, Ohio, November 20, 1997

106. Multimillion Atom Simulations of Sintering, Consolidation, and Fracture of High Temperature Materials on Parallel Computers
P. Vashishta, Workshop on "Computational Materials Physics in the Southeast", Vanderbilt University, Nashville, Tennessee, November 5-8, 1997.

107. Multimillion Atom Molecular Dynamics Simulations of Si/Si/Si3N4 Nanopixel-Structural Correlations at Si/Si3N4 Interface, Fracture, and Atomic Level Stresses in the Nanopixel
P. Vashishta, Workshop on "Interfacialy Controlled Functional Materials: Electrical and Chemical Properties", Schlob Ringberg, Germany, March 8-13, 1998.

108. Large-Scale Molecular Dynamics Simulations of Mechanical Properties of Ultrafine Microstructures on Parallel Computers
P. Vashishta, Symposium on "Computational and Mathematical Models of Microstructural

INVITED TALKS AT CONFERENCES:

Evolution", Materials Research Society Meeting, San Francisco, April 13-17, 1998.

109. Multimillion Atom Molecular Dynamics Simulations of Mechanical Properties of Nanostructures in
Ceramics and at Semiconductor/Ceramic Interfaces
P. Vashishta, Symposium on "Computational Modeling of Materials and Processing", American
Ceramic Society, Cincinnati, Ohio, May 3-6, 1998

110 Multimillion Atom Molecular Dynamics Simulations of Ceramic Materials and Interfaces on Parallel Computers
P. Vashishta, Fourth Special Symposium on "Advanced Materials", Nagoya, Japan, May 12-14, 1998.

111. Large-Scale Molecular Dynamics Simulations of Amorphous on Parallel Computers
P. Vashishta, CECAM workshop: "Intermediate Range Order in Network Forming Liquid and Glasses", Lyon, France, May, 18-20 1998.

112. Large Scale Simulations of Glasses on Parallel Computers: Nanophase Glasses and Ceramics
P. Vashishta, The 18th International Congress on Glass, San Francisco, CA, July 5-10, 1998.

113. Large Scale Computer Simulation of Glasses
P. Vashishta, Workshop on "Modeling Disordered Materials", American Crystallographic Society, Washington DC, July 18-24, 1998

114. Multimillion Atom simulations of Crack Propagation, Fracture, and Nanoindentation in Ceramic Materials
P. Vashishta, Gordon Conference on "High Temperature Materials, Processing, & Diagnostics", Plymouth, New Hampshire, July 19-24, 1998

115. Atomic Stresses in Si/Si3N4 Nanopixel - 10 Million Atom Molecular Dynamics Simulation on Parallel Computers
P. Vashishta, CECAM Workshop on "Surfaces and Interfaces far from Equilibrium", Lyon France, July 27-29, 1998

116. Atomic Stresses in Si/Si3N4 Nanopixel - 10 Million Atom Molecular Dynamics Simulation on Parallel Computers
P. Vashishta, "New Developments in High Temperature Ceramics", Istanbul, Turkey, August 12-15, 1998

117. Multimillion Atom Simulations of Silica: Crack Propagation and Fracture and Morphology of Fracture Surfaces in Amorphous Silica and Nanophase Silica
P. Vashishta, SILICA98, Mulhouse, France, September 1-4, 1998

118. Multimillion Atom Molecular Dynamics Simulations of Ceramic Materials and Interfaces on Parallel Computers
P. Vashishta, "Advanced Materials for Extreme Environments: New Experimental Opportunities
in Neutron Scattering", Argonne National Laboratory, Illinois, September 11-12, 1998

119. Multimillion Atom Simulation of Crack Propagation, Fracture, and Nanoindentation in Ceramic Materials
P. Vashishta, "Computational Studies of Interfacial Phenomena: nanoscale to Mesoscale" Pacific

INVITED TALKS AT CONFERENCES:

Northwest National Laboratory, Richland, Washington, September 24-25, 1998

120. Multimillion Atom Molecular Dynamics Simulations of Ceramic Materials and Stresses in Silicon/Silicon/Silicon Nitride Nanopixel
P. Vashishta, International Union of Materials Research Society, Banglore, India, October 13-16, 1998

121. Multimillion Atom Simulations of Crack Propagation, Fracture, and Nanoindentation in Ceramic Materials and Glasses
P. Vashishta, Symposium on "Fracture and Ductile vs Brittle Behavior -Theory, Modeling, and Experiments", Materials Research Society, Boston, MA, November 30-December 4, 1998

122. Multimillion Atom Simulation of Materials on Parallel Computers -Nanopixel and Nanoindentation
P. Vashishta, "Solid State Physics Symposium 1998", Kurukshetra, India, December 27-31, 1998

INVITED TALKS AT CONFERENCES:

123. Large Scale Atomistic Simulations of Ceramic Materials and Interfaces on Parallel Computers
P. Vashishta, "Thermo-Mechanical and Electrical Properties of High-Temperature Materials", Maui,January 4-9, 1999

124. Molecular Dynamics Simulations of Materials on Parallel Computers
P. Vashishta, "Scientific Simulation Initiative", Jefferson Nat'l Laboratory, VA, January 21, 1999

125. Multimillion Atoms Simulation of High Temperature Ceramic Materials
P. Vashishta, " The Kick-off Meeting for the Eutectic Research", National Science Foundation, Arlington, VA, February 24, 1999

126. Multimillion Atom Molecular Dynamics Simulations of Ceramic Materials and Interfaces on Parallel Computers
P. Vashishta, Symposium on "Spanning the Size Scales in Materials Phenomena", American Physical Society Centennial Meeting, Atlanta, Georgia, March 22-26, 1999

127. Crack Propagation and Fracture in Nanophase Materials - Multimillion Atom Molecular Dynamics
Simulation on Parallel Computers
P. Vashishta, "Nanocomposites: Design and Applications", Anchorage, Alaska, March 28-April 2, 1999

128. Multimillion Atom Simulations of Crack Propagation, Fracture, and Nanoindentation in Ceramic Materials
P. Vashishta, "High Strength Steels - Processing and Applications", Ranchi, India, April 14-15, 1999

129. Large Scale Materials Simulations on Parallel Computers
P. Vashishta, "Computational Materials Science Network on Ceramic/Polymer Interfaces", Sandia National Laboratory, Albuquerque, NM, April 22-23, 1999

130. Large Scale Simulations of Glasses on Parallel Computers: Nanophase Glasses and Ceramics
P. Vashishta, NATO Advanced Study Institute on "Physics of Glasses: Structure and Dynamics", Corsica, France, May 10-22, 1999

131. Computational Assisted Development of High Temperature Structural Materials
P. Vashishta, "DoD Challenge Workshop", Montrey, CA, June 6-10, 1999

132. Large Scale Simulations of Glasses on Parallel Computers: Nanophase Glasses and Ceramics
P. Vashishta, NATO Advanced Study Institute on "Physics of Glasses: Structure and Dynamics", Corsica, France, May 10-22, 1999

133. Multimillion Atom Molecular Dynamics Simulations of Ceramic Materials and Interfaces on Parallel Computers
P. Vashishta, "International Conference on Advanced Materials", Beijing, China, June 13-18, 1999

134. Multimillion Atom Simulations of Nanostructured Materials on Parallel Computers - Molecular Dynamics Method and Its Applications
P. Vashishta, "Computational and Applied Mathematics", St. Louis, MO, August 9-11, 1999

135. Atomistic Simulations of Nanoindentation of Silicon Nitride on Parallel Computers
P. Vashishta, "IMRC -Theory and Computer Simulation of Materials ", Cancun, Mexico, August 30-September 3, 1999

INVITED TALKS AT CONFERENCES:

136. Multimillion Atom Simulations of Nanostructured Materials on ParallelComputers - Sintering and Consolidation, Fracture, and Oxidation
P. Vashishta, "International Conference on Computational Physics ", Kanazawa, Japan, October 11-13, 1999

137. Atomistic Simulations of Nanostructures: Multimillion Atom Molecular Dynamics Simulations on ParallelComputers
P. Vashishta, "Foresight Conference on Molecular Nanotechnology ", San Jose, CA, October 15-17, 1999

138. Computational Assisted Development of High-Temperature Structural Materials
P. Vashishta, "Defense Science Board Presentation", Washington, DC, February 4, 2000

139. Multi-Million Atom Molecular Dynamics Simulations of Metal/Ceramic and Semiconductor/Ceramic Interfaces on Parallel Computers
P. Vashishta, "Workshop on Process Modeling of Laminated Multilayer Ceramic Systems", Motorola University,Tempe, Arizona, March 1, 2000

140. Molecular Simulations of Solids: Metals, Semiconductors, Ceramics, and Glasses
P. Vashishta, "International Comparative Study of Applications of Molecular and Materials Modeling", Washington, DC, March 14, 2000

141. Mulltimillion Atom Simulation of Nanostructured Materials on Parallel Computers – Sintering and Consolidation and Fracture and Oxidation
P. Vashishta, "The Materials Society (TMS)", Nashville, TN, March 12-16, 2000

142. Large-Scale Atomistic Simulations of Solid State Materials Modeling Many Millions of Atoms on Parallel Computers
P. Vashishta, "American Physical Society ", Minneapolis, March 22-24, 2000

143. Multimillion Atom Simulations of Materials on Parallel Computers - Past, Present and Future
P. Vashishta, "Celebrating the Success of LSU Computer Science" Baton Rouge, LA, April 14, 2000

144. Multimillion Atom Simulations of Nanophase Materials on Parallel Computers
P. Vashishta, "Seminars on Humanity 3000- Nanotechnology In the Future", Foundation for the Future, Bellevue, WA, April 21, 2000

145. Computer Simulations of Ceramic Interfaces
P. Vashishta, "AFOSR Meeting on Ceramic Materials and Composites" Saint Louis, MO, May 4-5, 2000

146. Multimillion Atom Simulations of Materials on Parallel Computers - Past, Present and Future
P. Vashishta, "XXIII Encontro Nacional de Física da Matéria Condensada", São Lourenço, Minas Gerais, Brasil, May 11-13, 2000

147. Multi-Million Atom Simulation of Sintering and Consolidation on Parallel Computers
P. Vashishta, "SIAM Conference on Mathematical Aspects of Materials Science", Philadelphia, PA, May 23, 2000

INVITED TALKS AT CONFERENCES:

148. Recent Research Activities in Material Sciences at LSU: Introduction to Concurrent Computing Laboratory for Materials Simulations (CCLMS)
P. Vashishta, "Niigata University-LSU Symposium", Niigata University, Niigata, Japan, May 30, 2000

149. Computational Assisted Development of High-Temperature Structural Materials
P. Vashishta, "DoD High Performance Computing Modernization Program Conference", Albuquerque, NM, June 5-8, 2000

150. Large-Scale Atomistic Simulations of Amorphous Polymers and Ceramic/Polymer Interfaces on Parallel Computers
P. Vashishta, "American CrystallographicSociety ", Minneapolis, MN, July 22-27, 2000

151. Multimillion Atom Simulation of Materials on Parallel Computers -Nanopixel, Interfacial fracture, Nanoindentation, and Oxidation
P. Vashishta, "MAPINT Symposium on Multidisciplinary Applications and Interoperable Computing", Dayton, Ohio, August 17, 2000

152. Atomistic Modeling Capabilities for Sintering of Ceramics and Fracture at Interfaces
P. Vashishta, "NSF Multi-University I/UCRC Ceramic and Composite Materials Center", Piscatway, NJ, September 27-28, 2000

153. Multimillion Atom Simulation of Nanostructured Materials – Dynamic Fracture, Nanoindentation, and Oxidation
P. Vashishta, "International Conference on Engineering & Technological Sciences 2000 – Advanced Materials", Beijing, China, October 10-14, 2000

154. Large Scale Molecular Dynamics Simulations of Materials on Parallel Computers
P. Vashishta, "ACAT2000 Conference", Fermilab, IL, October 18-19, 2000

155. Large Scale Molecular Dynamics Simulations of Nanostructured Materials on Parallel Computers– Dynamic Fracture, Nanoindentation, and Oxidation
P. Vashishta, "Joint CNRS (France)-NSF (USA) Nanomaterials Workshop – Nanomaterials Toward Engineering Applications", Montreal, Canada, October 20-25, 2000

156. Multimillion Atom Simulation of Nanostructured Materials and Devices on Parallel Computers
P. Vashishta, "DAE Solid State Physics Symposium", Guru Ghasidas University, Bilaspur, India, December 27 - 31, 2000

157. Periodic Array of Stress Domains in Silicon/Silicon Nitride Nanopixels: A Multimillion Atom Molecular Dynamics Simulation
P. Vashishta, "International Conference on Science and Technology of Nanostructured Materials", Puri, India, January 8-12, 2001

158. Multimillion Atom Simulation of Materials on Parallel Computers - Nanopixel, Interfacial Fracture, Nanoindentation, and Oxidation
P. Vashishta, "Golden Jubilee of Saha Institute of Nuclear Physics", Calcutta, India, February 5-8, 2001

159. Multimillion Atom Simulation of Nanosystems at the Forefront of Information Technology and Nanosciences, and An Integrated Dual Degree Program of Research and Education
P. Vashishta, "National Science Foundation Distinguished Lecture", Arlington, VA, February 26, 2001

INVITED TALKS AT CONFERENCES:

160. Multimillion Atom Simulations of Mechanical Behavior of Nanostructured Materials, Interfaces, and Dynamics of Oxidation
P. Vashishta, "The Society of Materials Science, Japan (JSMS)", Osaka, Japan, May 21-26, 2001

161. Hybrid Atomistic -Continuum Simulations of Nanopixels: A Multimillion Atom Molecular Dynamics Simulation
P. Vashishta, "DoD High Performance Computing", Biloxi, MS, June 18-20, 2001

162. Multimillion Atom Simulations of Materials at the Forefront of Information Technology and Nanosciences
P. Vashishta, National Research Council, National Materials Advisory Board Meeting on "Materials Research for Defense-After-Next", Woods Hole Center of the National Academy of Sciences, MA, June 27-28, 2001

163. Massively Parallel Atomistic Simulations of Nanoparticles Under Extreme Conditions
P. Vashishta, "DARPA HEDAM/NANO Workshop", Rosslyn, VA, August 6-8, 2001

164. High Temperature Materials Simulations on Parallel Computers
P. Vashishta, "Joint Annual Review of AFOSR Metallic and Ceramic Materials Program", Snowbird, UT, August 19-21, 2001

165. High Performance Computing and Visualization: Opportunities and Challenges at the Information-Bio-Nano- Interface
P. Vashishta, "Frontiers in Information Technology", Rensselaer Polytechnic Institute, Troy, NY, November 8, 2001

166. Multimillion Atom Simulations of Nanosystems on Parallel Computers
P. Vashishta, "International Workshop on Condensed Matter Theories", Canberra, Australia, December 3-8, 2001

167. High Performance Computing and Visualization: Opportunities and Challenges at the Information-Bio-Nano Interface
P. Vashishta, "Computational Sciences Workshop for Underrepresented Groups", Baton Rouge Louisiana, January 6, 2002

168. Computational Materials Science on Teraflop-to-Petaflop Computers
P. Vashishta, "DOD, DOE, NASA Joint Conference on Mission Critical Computing", Washington DC, February 4-6, 2002

169. Multimillion Atom Simulations of Nanosystems on Parallel Computers
P. Vashishta, "International Symposium on Computational Science & Engineering", Tokyo, Japan, March 5-6, 2002

170. Large-Scale Molecular Dynamics Simulations of the Oxidation of Metallic Nanoparticles
P. Vashishta, "Gordon Conference on Energetic Materials", Tilton, NH, June 19, 2002

171. Billion-atom Multiscale Simulations on a Grid
P. Vashishta, "NSF DMR Computational Materials Theory Program Review", Urbana, IL, June 20, 2002

172. Amorphous Materials in Various Incarnations

INVITED TALKS AT CONFERENCES:

P. Vashishta, "CECAM Workshop on Atomic Structure and Transport in Glassy Networks", Lyon, France, June 24-27, 2002

173. Multimillion Atom Simulations of Nanosystems on Parallel Computers - Nanopixel, Nanoindentation and Oxidation
P. Vashishta, "APS Conference on Computational Physics 2002", San Diego, August 25-28, 2002

174. Multimillion Atom Simulations of Nanosystems on Parallel Computers - Nanopixel, Nanoindentation and Oxidation of Aluminum Nanoparticles
P. Vashishta, "CNER-MSI Nanosimulation Workshop" Center for NanoEnergetics Research Minnesota Supercomputing Institute, Minneapolis, MN, August 26-27, 2002

175. Info-Bio-Nano Interface: High-Performance Computing & Visualization
P. Vashishta, "High Performance Computing 2002", Bangalore, India, December 18-21, 2002

176. Info-Bio-Nano Interface: High-Performance Computing & Visualization
P. Vashishta, "Computational Science Workshop for Underrepresented Groups", LSU@Baton Rouge, LA, January 5-11, 2003

177. Large Scale Atomistic Simulations of Reactivity of Nanosystems - Nanostructured Materials and Oxidation of Aluminum Nanoparticles
P. Vashishta, "Expanding the Envelope: Nano Materials for Aerospace Symposium" Corpus Christi, Texas, January 27-30, 2003

178. Multimillion Atom Simulation of nanosystems on Parallel Computers – nanophase Material, Nanopixel, Nanoindentation and Oxidation
P. Vashishta, "Modeling and Simulations in Micro and Nano Technologies and Materials Engineering, Toulouse, France, April 7-11, 2003

179. Multimillion Atom Simulations of Nanosystems and Interfaces on Parallel Computers
P. Vashishta, "International Conference on Non-Crystalline Inorganic Materials-Synthesis, Structure and Simulation: CONCIM", Bonn, Germany, April 8-12, 2003

180. Multimillion Atom Molecular Dynamics Simulations of Nanostructures on Parallel Computers
P. Vashishta, "International Conference on Computational Engineering & Science", Corfu, July 25, 2003

181. Multimillion Atom Molecular Dynamics Simulations of Nanostructures on Parallel Computers
P. Vashishta, "High-Tech Conference, Inha University and University of Southern California Korea" September 17-18, 2003

182. Multimillion Atom Molecular Dynamics Simulations of Nanostructured Materials
P. Vashishta, "Symposium on Multiscale Design of Nano-materials, IUMRS-ICAM2003", Yokohama, Japan, October 10-11, 2003

183. Multimillion Atom Molecular Dynamics Simulations of Nanostructures on Parallel Computers
P. Vashishta, "International Conference on Nanoscience & Technology, ICONSAT 2003", Kolkata, India, December 17-20, 2003

184. Multimillion Atom Simulations of Nanosystems and Billion Atom Walkthrough,
Priya Vashishta, "N+N Program", Washington, DC, April 15-16, 2004

185. Multimillion Atom Molecular Dynamics Simulations of Nanostructures on Parallel Computers
Priya Vashishta, "Computational Science Workshop for Underrepresented Groups", University of Southern California, 5-10January, 2004

186. Atomistic Simulations on High-end Computers and Billion Atom Walkthrough

INVITED TALKS AT CONFERENCES:

Priya Vashishta, "Research Opportunities in Cyberengineering/Cyberinfrastructure", Drexel, April 22-23, 2004

187. Multimillion Atom Molecular Dynamics Simulations of Nanostructures on Parallel Computers
Priya Vashishta, "Atomic Scale Materials Design; Modeling and Characterization", E-MRS Spring Meeting, Strasbourg, France, May 24-28, 2004

188. Multimillion Atom Simulations of Nanosystems and Interfaces on Parallel Computers
Priya Vashishta, Inaugural Session, 3rd International Conference "Computational Modeling & Simulation of Materials", Acireale, Sicliy, Italy, May 30-June 4, 2004

189. Billion-atom Multiscale Simulations of Nanosystems on a Grid
Priya Vashishta, NSF Division of Materials Research ITR Computational Workshop University of Illinois, Urbana, June 17-19, 2004

190. Ultrascale Simulations High Performance Computing and Visualization
Priya Vashishta, Metaphoric Optical Computing Workshop San Diego, CA, July 12, 2004

191. Large-Scale Atomistic Simulations of Nanosystems on Parallel Computers
Priya Vashishta, "International Conference on Computational Engineering & Science", Madeira, Portugal, July 26-29, 2004

192. Multimillion Atom Simulations and Visualization of Oxidation and Hypervelocity Impact Damage
Priya Vashishta, "Advanced Computing and Simulation", 24th Army Science Conference, Orlando, FL, November 30, 2004

193. Multimillion Atom Simulations of Dynamics of Oxidation of an Aluminum Nanoparticle and Hypervelocity Impact Damage in AlN Ceramic,
Priya Vashishta, "Michael Klein 65th Birthday Symposium", ACS Meeting, San Diego, CA, March 13-17, 2005

194. Multimillion Atom Simulations of Nanosystems: Structural Transformation in Nanocrystals and Hypervelocity Impact Damage
Priya Vashishta, "Algorithm and Software Developments in Nanoscale Simulations" RISC_AIST Computational Science Workshop, Tsukuba, Japan March 22-23, 2005

195. Multimillion Atom Simulations of Hybrid Nanosystems
Priya Vashishta, "Hybrid Molecular/ Semiconductor Structures: Design of Electronics by Computation", ARO/AFOSR Workshop, Rosslyn, Virginia, June 17, 2005

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

197. Multimillion Atom Simulations of Nanostructured Materials on Parallel Computers
Priya Vashishta, "5th International Congress of Theoretical Chemical Physics", New Orleans, LA, July 20-26, 2005

198. Multimillion Atom Simulations of Materials Dynamics of Oxidation & Mechanical Behavior on Parallel Computers
Priya Vashishta, Workshop on "Modeling Materials in Extreme Environment (ME2)", Washington DC, September 24-25, 2005

199. Multimillion Atom Simulations of Nanosystems - Structural Transformations in Nanocrystals, Dynamics of Oxidation, and Hypervelocity Impact Damage
Priya Vashishta, Workshop on "Multiscale Modeling in Condensed Matter and Materials Science." Institute for Pure and Applied Mathematics (IPAM), UCLA, October 17-20, 2005

INVITED TALKS AT CONFERENCES:

200. Multiscale Algorithms for Multimillion Atom Simulations on Parallel Computers
Priya Vashishta, "International Conference on Computational & Experimental Engineering & Sciences (ICCES05) ", Chennai, India, December 1-6, 2005

201. Multimillion Atom Simulations - Oxidation of Aluminum Nanoparticles, Nanophase materials, and Hypervelocity Impact Damage
Priya Vashishta, U. S. ARMY Materials Summit "Disruptive Materials Technology", Gettysburg, PA, March 14, 2006

202. Multimillion Atom Simulations of Nanostructured Materials on Parallel Computers
Priya Vashishta, "HPC Forum", Richmond, VA, April 12, 2006

203. Multimillion Atom Simulations of Reactive Nanosystems on Parallel Computers
Priya Vashishta, "11th international Ceramics Congress and 4th Forum on New Materials", Acireale, Sicily, June 4-9, 2006

204. Multimillion Atom Simulations of Dynamics of Wing Cracks and Hypervelocity Impact Damage
Priya Vashishta, " Nano-Technology and Information Technology for Space Applications", Pasadena Conference Center, Pasadena, CA, July 16, 2006

205. Multimillion Atom Simulations of Dynamics of Wing Cracks and Hypervelocity Impact Damage
Priya Vashishta, "Multiscale Nano- and Bio-Mechanics and Materials", 7th World Conference on Computational Mechanics (WCCM), Los Angeles, CA, July 16-22, 2006

206. Multimillion Atom Simulations of Dynamics of Wing Cracks and Nanoscale Damage in Glass, and Hypervelocity Impact Damage in Ceramics
Priya Vashishta, "The 12th International Symposium on Plasticity & Its Applications", Halifax, Canada, July 17-22, 2006

207. Multimillion Atom Simulations of Dynamics of Wing Cracks and Nanoscale Damage in Glass, and Hypervelocity Impact Damage in Ceramics
Priya Vashishta, "Conference on Computational Physics", Gyeongju, Republic of Korea, August 29-September 1, 2006

208. Multimillion Atom Simulations of Nanoscale Materials on Parallel Computers
Priya Vashishta, "APS California Section Meeting", CSU, Long Beach, October 27-28, 2006

209. Multimillion Atom Simulations of Nanosystems on Parallel Computers
Priya Vashishta, Chile Physical society, Santiago, Chile, November 15,-17 2006

210. Multimillion Atom Simulations of Nanosystems on Parallel Computers
Priya Vashishta, "Physics of Mesoscopic and disordered Materials", IIT Kanpur, India, December 4-8, 2006

211. Thermal Management Strategic Technology
Priya Vashishta, "Air Force Research Laboratory Workshop", Dayton, Ohio, March 29, 2007

212. Multimillion Atom Simulations of Nanostructured Materials
Priya Vashishta, "5th International Symposium on Theory of Atomic and Molecular Clusters ", Richmond, Virginia, May 17, 2007

213. Multimillion to Billion Atom Simulations of Nanostructured Materials Under Extreme Conditions
Priya Vashishta, "Multi-scale and Large-scale Simulations in DoD Materials Science", Mitre Corporation, Mclean, Virginia, June 14-15, 2007

214. Multimillion to Billion Atom Simulations of Materials
Priya Vashishta, "Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday", ACS Meeting, Boston, Mass, August 22, 2007

INVITED TALKS AT CONFERENCES:

215. Multimillion to Billion Atom Simulations of Nanostructured Materials Under Extreme Conditions
Priya Vashishta, "Dreams, Creation and Realization of Materials Saving the Humankind",
17th IKETANI International Conference, Tokyo, Japan, September 5-8, 2007

216. Multimillion to Billion Atom Simulations of Nanostructured Materials Under Extreme Conditions
Priya Vashishta, "Ultrascale Hierarchical Simulations on High-End Parallel and Distributed Computers" , APCOM'07-EPMESC XI, Kyoto, Japan, December 03, 2007

217. Multimillion to Billion Atom Simulations of Reactive Nanosystems
Priya Vashishta, "Workshop on Pseudopotentials and Complex Materials",
Jim Chelikowsky's 60th Birthday Celebration, Austin, Texas, April 10-11, 2008

218. Multimillion to Billion Atom Simulations of Nanosystems Under Extreme Conditions
Priya Vashishta, "Fragmentation Processes in the Earth" , The 21st Kronsberg Seminar,
Norway, May 7-9, 2008

219. Multimillion to Billion Atom Simulations of Nanoenergetic Materials
Priya Vashishta, "Microthermal Initiator & NanoEnergetic Device Workshop",
Army research Laboratory, Adelphi, MD, May 22-23, 2008

220. Multimillion Atom Simulations of Energetic Materials: Combustion of Al Nanoparticles and Reactive Nanojets in Nanostructure-Enhanced Chemical Reactions
Priya Vashishta, "Gordon Conference on Energetic Materials", Tilton, NH, June 15-20, 2008

221. Multimillion to Billion Atom Simulations of Nanostructured Materials Under Extreme Conditions
Priya Vashishta, "The 1 st International Symposium on Advanced Microscopy and Theoretical Calculations", Nagoya, Japan, June 29-30, 2008

222. Multimillion to Billion Atom Simulations of Reactive Nanosystems and Stress Corrosion
Priya Vashishta, "Corrosion – Aqueous: Mechanisms, Methods and Models",
Colby-Sawyer College, New London, NH, July 20-25, 2008

223. Multimillion to Billion Atom Simulations of Nanosystems Under Extreme Conditions
Priya Vashishta, "Conference on Current Trends in Computational Chemistry 2008",
Jackson, MS, October 30 - November 1, 2008

224. Multimillion to Billion Atom Simulations of Nanosystems Under Extreme Conditions
Priya Vashishta, "Computational Approaches and Applications in Earth Materials Studies",
American Geophysical Union, San Francisco, CA, December 15-19, 2008

225. High Performance Computing for Billion Atom Simulations of Nanosystems
Priya Vashishta, "Scientific Discovery through Advanced Computing", ICCES'2009,
Phuket, Thailand, April 8, 2009

226. Multimillion Atom Simulations of Reactive Nanosystems
Priya Vashishta, "Symposium on Nano-scale Energetic Materials: Fabrication, Characterization and Molecular Modeling", E-MRS 2009 Spring Meeting, Strasbourg, France, June 8-12, 2009

227. Multimillion to Billion Atom Simulations of Nanostructured Materials Under Extreme Conditions
Priya Vashishta, "Symposium in Honor of Professor Sidney Yip", USNCCM 10,
Columbus, OH, July 16-18, 2009

228. Multimillion Atom Simulations of Reactive Nanosystems
Priya Vashishta, "International Workshop on Condensed Matter Theories: CMT-33", Quito,
Ecuador, August 16-21, 2009

229. Fast Reaction Mechanism of Al/Al_2O_3 Nanoparticles in Oxygen: Multimillion Atom Simulations of Nanoenergetic Materials
Priya Vashishta, "Advancements in Energetic Materials & Chemical Propulsion", 8-ICICP,
Cape Town, South Africa, November 2-6, 2009

INVITED TALKS AT CONFERENCES:

230. Multimillion Atom Simulations of Nanostructured Materials
Priya Vashishta, "CIFAR Nanoelectronics Meeting", Quebec, Canada, November 16, 2009

232. Multimillion Atom Simulations of Reactive Nanosystems
Priya Vashishta, "Multiscale Modeling and Simulations of Hard and Soft Materials", JNCASR, Bangalore, India, December 17-20, 2009

233. Multimillion Atom Simulations of Reactive Nanosystems
Priya Vashishta, "Plasticity 2010", St. Kitts, January 3-8, 2010

234. Hydrogen Production from Water Using Aluminum Superatoms
Priya Vashishta, "Theory of Atomic & Molecular Clusters (TAMC VI)", Mexico City, Mexico, June 13-17, 2010

235. Material Properties and Processes Using High Performance Computing
Priya Vashishta, "Supercomputing: The Imperative and the Path Forward", New York University Abu Dhabi Institute, Abu Dhabi, January 9-10, 2011

236. Computational Tools: Current length and time scales Petascales to Exascale Computing
Priya Vashishta, "Workshop on Harnessing DOE's High Performance Computing Expertise to Strengthen the US Chemical Enterprise", Council for Chemical Research and Department of Energy, Washington DC, March 10, 2011

237. Reactive Nanosystems
Priya Vashishta, "3rd International Conference from Nanoparticles and Nanomaterials to Nanodevices and Nanosystems", IC4N-2011, Crete, Greece, June 26, 2011

238. Multimillion to Billion Atom Simulations of Properties and Processes in Materials
Priya Vashishta, "8th International Conference on Diffusion in Materials (DiMat 2011)", Dijon, France, July 4-8, 2011

239. Multimillion to Billion Atom Simulations of Properties and Processes in Materials
Priya Vashishta, "High Fidelity 3D Multiscale Materials Modeling and Experimental Analysis Workshop", Vicksburg, MS, August 2–3, 2011

240. Reactive Nanosystems: Multimillion Atom Molecular Dynamics Simulations of Energetic Materials
Priya Vashishta, "Workshop on Nanoenergetics and Combustion Dynamics", Arlington, Virginia, August 23-25, 2011

241. Multimillion to Billion Atom Simulations of Properties and Processes in Materials
Priya Vashishta, "Materials Science and Technology (MS&T 2011)", Columbus, OH, October 14, 2011

242. Multimillion Atom Simulations of Reactive Nanosystems
Priya Vashishta, "The International Workshop on the Physics of Semiconductor Devices", IIT Kanpur, India, December 19-22, 2011

243. Multimillion Atom MolecularDynamics Simulations of Reactive Nanosystems
Priya Vashishta, "PACAM XII", Port of Spain, 2-6 January 2012

244. Shock Compression of Condensed Systems: Role of Emerging Computing Platforms
Priya Vashishta, "Dynamic Compression Sector @ APS User Workshop", 19-20 January 2012

INVITED TALKS GIVEN AT UNIVERSITIES AND RESEARCH ORGANIZATIONS:

St. Andrews University, U. K. (1968)
McMaster University, Canada (1970, 1983)
Dalhousie University, Canada (1970)
Northwestern University (1971)
Iowa State University (1972)
Michigan State University (1972, 1994)
IBM Thomas J. Watson Research Center- Yorktown (1972)
Argonne National Laboratory (1972, 1974, 1978, 1981, 1985, 1989. 1991, 1994)
Western Michigan University (1973, 1979)
University of Messina, Italy (1973, 1973)
Roorkee University, India (1973)
Tata Institute of Fundamental Research, India (1973)
Northern Illinois University (1974, 2005)
University of Iowa (1974)
University of Chicago (1974, 1982)
University of Cincinnati (1974)
University of Illinois at Chicago (1974, 1982)
University of California - Berkeley (1975, 1982)
University of British Columbia, Canada (1975, 1983)
Osaka University, Japan (1975, 1985)
Nagoya University, Japan (1975, 1975, 1985)
Purdue University (1975, 1978, 1981, 1984)
Bell Laboratory - Holmdel (1976)
University of California - San Diego (1977, 1977, 1982, 2011)
University of California - Los Angeles (1977, 2004)
University of California - Davis (1977, 2004, 2011)
CECAM - Orsay, France (1977)
University of Missouri - Columbia (1978, 1983, 1984)
University of Illinois - Urbana (1979)
Chalmers Institute of Technology, Sweden (1981, 1981)
Western Illinois University (1981)
Arizona State University (1981)
Bell Laboratories - Murray Hill (1981)
Brown University (1981)
Cornell University (1981, 1987)
IBM Research Laboratory - San Jose (1982)

INVITED TALKS GIVEN AT UNIVERSITIES AND RESEARCH ORGANIZATIONS:

Washington University - St. Louis (1982, 1984, 1991)
California Institute of Technology (1982)
University of Minnesota (1982, 1988)
University of California - Irvine (1982, 2011)
University of Southern California (1982, 2001, 2003)
University of Toronto - Canada (1983)
Simon Fraser University - Canada (1983)
Institute for Theoretical Physics - Santa Barbara (1983, 1994)
University of Houston, Houston, TX (1983, 1996))
Kansas State University (1984)
International Center for Theoretical Physics - Trieste, Italy (1984)
Schlumberger-Doll Research Laboratory (1984)
Institute of Solid State Physics, Tokyo, Japan (1985, 1989)INVITED
Tokyo University, Japan (1985, 1989)
Kyoto University, Japan (1985, 1989)
Niigata University, Japan (1985, 1989, 2007)
Tohoku University, Japan (1985, 1989)
University of Sao Paulo, Sao Carlos, Brazil (1985, 1987)
Louisiana State University (1988, 1989)
Australian National University, Canberra, Australia (1989)
Okayama University, Japan (1989, 1995)
Kanazawa University, Japan (1989)
Clemson University (1990)
Panjab University, India (1991)
National Physical Laboratory, India (1991)
Institute of Physics - Bhubaneswar, India (1991)
Indian Institute of Science - Bangalore, India (1991)
Emory University (1991)
Texas A&M University (1991)
Minnesota Supercomputing Research Institute (1991)
NEC Corporation, Tsukuba, Japan (1992)
Government Industrial Research Institute, M I T I, Osaka, Japan (1992)
University of New South Wales, Sydney, Australia (1993)
Institute of Advanced Study, Canberra University, Canberra, Australia (1993)
National Institute for Standards and Technology (NIST), Washington DC (1994)
Energy Research Laboratory, Hitachi City, Japan (1994)

INVITED TALKS GIVEN AT UNIVERSITIES AND RESEARCH ORGANIZATIONS:

Argonne National Laboratory, Argonne, IL (1996)
Northwestern University, Evanston, IL (1996)
Institute of Theoretical Physics, Unversity of California, Santa barbara (1997)
Argonne National Laboratory, Argonne, IL (1997)
NASA Ames Laboratory, CA (1997)
Ohio State University, Columbus, OH (1997)
Rice University, Houston, TX (1998)
Ohio State University (1998)
Cornell University, Ithaca, NY (1999)
Florida State University, Tallahassee, FL (2000)
Harvard University, Cambridge, MA (2000, 2008)
Universidade Federal de São Carlos, São Carlos, Brasil (2000)
Universidade Federal (UFAL), Maceio, Brasil (2000)
North Carolina State University, NC (2000)
Livermore National Laboratory, CA (2001)
General Motors, MI (2001)
Fermi National Laboratory, IL (2001)
University of Georgia, GA (2001)
Sandia National Laboratory (2001)
Agilent Technologies, CA (2003)
Army Research Laboratory, Aberdeen Proving Grounds, MD (2004)
University of Pittsburgh, PA (2007)
University of Uppsala, Uppsala, Sweden (2009)
University of South Florida, Tempa, Florida (2011)