Panchapakesan Ganesh

Research & Development Associate Staff Member
Center For Nanophase Materials Sciences Division
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Education

Carnegie Mellon University, USA	Physics	MS/PhD, 2007
University of Pune, Pune, India	Physics	MSc., First-Class, 2002
Presidency College, Calcutta, India	Physics	B.Sc. with Hons, 2000

Professional Experience (ORNL = Oak Ridge National Laboratory; CIS = Carnegie Instituion for Science; CMU = Carnegie Mellon University)

2010 – present	R&D Associate Research Staff, Center for Nanophase Materials Sciences, ORNL
2010 – 2012	FIRST-EFRC Fellow, Center for Nanophase Materials Sciences, ORNL
2007 – 2010	Postdoctoral Research Associate, Geophysical Laboratory, CIS
2006 – 2007	The Joseph A. Kane Research Fellow, Department of Physics, CMU
2005 – 2006	The George E. and Majorie S. Pake Fellow, Mellon College of Science, CMU
2002 – 2005	Research and Teaching Assistant, Department of Physics, CMU

Professional and Synergistic Activities

2011–present	Active referee, American Chemical Society Journals
2006–present	Active referee, American Physical Society and American Institute of Physics Journals

Honors and Awards

2010 – 2012	FIRST-EFRC Fellowship, ORNL
2006 – 2007	The Joseph A. Kane Research Fellow, Department of Physics, CMU
2005 – 2006	The George E. and Majorie S. Pake Fellow, Mellon College of Science, CMU

Publications (Around 20 publications including 1 book chapter)
Full publication list follows CV.

Research Synopsis
Current Projects:

1. *Develop atomistic models and fundamental understanding of Li/Na-ion batteries.*
   We use a wide range of methods, from quantum monte-carlo to electronic density functional theory to classical reactive- and non-reactive force-field modeling to simulate and understand the structure, dynamics and reactions in Li- and Na-ion battery materials, in a wide range of length- and time-scales. The current focus is in understanding electrolytes and their interfaces with electrodes as well as in employing a combination of structure finding methods to understand conversion electrodes with the aim of optimizing energy and power density with minimum capacity loss for thousands of cycles.
2. *Establish an understanding of graphene-based solid-fluid interphases for supercapacitance and catalysis applications.*
   We use a range of methods from ab initio molecular dynamics to reactive force-field simulations to

understand the interactions of fluids (such as water) with epitaxial graphene and carbon-nanostructures. The current focus is in understanding and quantifying key control parameters (defects, epitaxial-strain, functionalization etc.) which determine interfacial atomic structure and charge-transfer, on experimentally verified structural models that we build.

3. *Establish an absolute understanding of fluid-mediated catalysis on oxide supported nanoparticles*
We use electronic density functional theory based methods to understand the role of water in mediating technologically important reactions on oxide (TiO_2, ZrO_2 etc.) supported gold nanoparticles. The previous focus in in understanding and quantifying the role of surface hydroxyls on reaction pathways and kinetics. Currently the role of interfacial water in direct mediation of technologically important surface reactions is being investigated with high level theory.

4. *Understand and predict new and improved multiferroic materials, both in bulk and thin-filmgeometries, for various electronic and energy harvesting applications*

   We employ a combination of high level electronic structure theory, effective Hamiltonian methods and structure prediction methods to predict bulk and thin-film properties of multiferroic materials. We work closely with experimentalists at CNMS to synthesize and characterize them, to build a coherent understanding of the origin of their novel properties.

5. *Investigation of superconductivity and other emergent behavior in organic superconductors when interfaced with solids*

   Origin of strong electronic correlations and resulting superconductivity in 3-dimensional organic superconductors opens the possibility of their controlled growth and characterization on solid surfaces with characteristic electronic properties (metals, insulators, topological insulators etc.). Understanding the emergent correlated electron physics at the nanoscale at solid-molecule interfaces should allow us to engineer superconducting materials bottom-up. We employ a range of high-level electronic structure methods to investigate this in conjunction with experiments and theory experts in strongly correlated methods at CNMS.

Previous Projects:

1. *Phase transitions in solids under pressure*
   I used solid state electronic structure calculations, phonons and *ab initio* molecular dynamics to elucidate novel phase transitions in a wide range of perovskite ferroelectrics, relaxors and magnetic mineral-oxides. Bulk, thin-films and superlattices were studied in many cases. The effort was later extended to study molecular compound formation with hydrogens under pressure. Several new materials and phenomenologies were predicted and verified with experiments.

2. *Phase transitions in supercooled liquid silicon*
   I used *ab initio* molecular dynamics with statistical-mechanics and thermodynamics to predict liquid-liquid phase transitions in atomic silicon in its supercooled regime. Our predictions were later supported by experiments.

3. *Geometric frustration and glass-formability in metallic glass*
   I used *ab initio* molecular dynamics with statistical-mechanics to understand and predict the relation between geometric frustration in atomic structure and glass formability in metallic glasses.

PATENTS

2011 New Class of Pure Piezoelectric Materials (U. S. Patent No. 8.039,131 B2)

LIST OF INVITED TALKS AND PUBLICATIONS

INVITED TALKS

2011 *"Accurate static and dynamic properties of electrolytes for Li-ion battery applications"*, P. Ganesh, Fall Meeting of the American Chemical Society, Denver, USA

2011 *"Origin of diffuse scattering in relaxor ferroelectrics"*, P. Ganesh, March Meeting of the American Physical Society, Dallas, USA

2010 *"Origin of diffuse scattering in relaxor ferroelectrics"*, P. Ganesh, Advances in the Fundamental Physics of Ferroelectrics and Related Materials, Aspen Center for Physics, Aspen, USA

2009 *"Liquid-liquid transition in supercooled liquid Si"*, P. Ganesh and M. Widom, (6th International Discussion Meeting on Relaxations in Complex Systems (IDMRCS)), Rome, Italy

PEER-REVIEWED PUBLICATIONS (ACCEPTED OR UNDER REVIEW)

- Over **300 citations** with an **h-index of 7**
- Publications in **Nature**, **PNAS**, **Phys. Rev. Lett.** and **J. Phys. Chem. Lett.** journals
  (A '' indicates sharing of first-/corresponding- authorship)*

1) *"Spin Resolved Self Doping Tunes the Intrinsic Half-Metallicity of AlN Nanoribbons"*, Alejandro Lopez-Bezanilla*, P. Ganesh*, P. R. C. Kent and Bobby G. Sumpter, **submitted to Phys. Rev. Lett. (2013)**

2) *"Catalytic CO Oxidation by Gold Nanoparticles Supported on Hydroxylated Zirconia"*, Christopher J.Karwacki, Gregory W. Peterson, Jun Jie Niu, P. Ganesh, P. R. C. Kent and Yury Gogotsi, **submitted to J. Phys. Chem. C (2012)**

3) *"Characterization of Sodium Ion Electrochemical Reaction with Tin Anodes"*, Loic Bagetto, Roberta Meissner, P. Ganesh, Raymond Unocic, Craig Bridges, Jean-Claude Dumas and Gabriel Veith, **submitted to Journal of Power Sources (2012)**

4) *"Solid−Electrolyte Interphase Formation and Electrolyte Reduction at Li-Ion Battery Graphite Anodes: Insights from First-Principles Molecular Dynamics"*,P. Ganesh, P. R. C. Kent and De-en Jiang, **J. Phys. Chem. C 116, 24476 (2012)**

5) *"Understanding Controls on Interfacial Wetting at Epitaxial Graphene:Experiment and Theory"*, H. Zou*, P. Ganesh*, V. Presser, M. C. F. Wander, Paul Fenter, P. R. C. Kent, De-en Jiang, Ariel Chialvo, J. McDonough, K. Shuford and Yuri Gogotsi, **Phys. Rev. B 85, 035406 (2012)**

6) *"Crystal Structures of $(Mg_{1-x},Fe_x)SiO_3$ Post-Perovskite at High Pressures"*, T. Yamanaka, K. Hirose, W. Mao, Y. Meng, P. Ganesh, L. Shulenburger, G. Shen, Russell J. Hemley, **PNAS 10, 1073 (2012)**

7) *"New Compound Formation and Hydrogen-Bonding Enhancement and Ordering in H_2S-H_2"*, T. Strobel*, P. Ganesh*, P. R. C. Kent and Russell J. Hemley, **Phys. Rev. Lett. 107, 255503 (2011)**

8) *"Role of Hydroxyls on the Adsorption and Activity of Au Nano-Particles on Rutile Surface"*, P. Ganesh, P. R. C. Kent and G. M. Veith, **J Phys. Chem. Lett. 2, 2918 (2011)**

9) *"Formation, Characterization and Dynamics of Multi-Shell Carbon Nano-Structures for Supercapacitors from Nano-Diamonds using Reactive Force-Fields"*, P. Ganesh, P. R. C. Kent and V. Mochalin, **J of Appl. Phys. 110, 073506 (2011)**

10) *"Accurate Static and Dynamic Properties of Liquid Electrolytes for Li-ion Batteries from ab initio Molecular Dynamics"*, P. Ganesh, De-en Jiang and P. R. C. Kent, **J. Phys. Chem. B 115, 3085 (2011)**

11) *"Orbital-Ordering, Ferroelasticity and the Large Pressure Induced Volume Collapse in $PbCrO_3$"*, P. Ganesh and R. E. Cohen, **Phys. Rev. B 83, 172102 (2011)**

12) *"Origin of Diffuse Scattering in Relaxor Ferroelectrics"*, P. Ganesh, E. Cockayne, M. Ahart, R. E. Cohen, B. Burton, Russell J. Hemley, Yang Ren, Wenge Yang and Z.-G. Ye, **Phys. Rev. B 81, 244102 (2010)**

13) *"First Principles Coexistence Simulations of Supercooled Liquid Silicon"*, P. Ganesh and M. Widom, **Journal of Noncrystalline Solids 357, 442 (2010)**

14) *"Liquid-Liquid Transition in Supercooled Silicon Determined by First-Principles Simulation"*, P. Ganesh and M. Widom, **Phys. Rev. Lett. 102, 075701 (2009)** (chosen as "Editor's Suggestion")

15) *"Finite-Electric Field Study of Pressure Effects on Polarization Rotation in $PbTiO_3$"*, P. Ganesh and R. E. Cohen, **MRS 2009 Fall Proceedings** (1199, 1199-F11-06 doi:10.1557/PROC-1199-F11-06)

16) *"First Principles Simulation of Supercooled Liquid Alloys"*, M. Widom, P. Ganesh, S. Kazimirov, D. Louca and M. Mihalkovič, **J. Phys. Condens. Matter 20, 114114 (2008)**

17) *"Search for New Piezoelectrics"*, P. Ganesh and R. E. Cohen, **MRS 2008 Fall Proceedings** (1110, 1110-C01-07 doi:10.1557/PROC-1110-C01-07)

18) *"Origin of Morphotropic Phase Boundaries in Ferroelectrics"*, M. Ahart, M. Somayazulu, R. E. Cohen, P. Ganesh, P. Dera, H.-K. Mao, Russell J. Hemley, Yang Ren, Peter Liermann and Zhigang Wu, **Nature 451, 545 (2008)**

19) *"Pressure Induced Phase Transition in $PbTiO_3$"*, P. Ganesh and R. E. Cohen, **J. Phys: Condens. Matter 21, 064225 (2008)**

20) *"Ab initio Simulations of Geometric Frustration in Supercooled Liquid Fe and Fe-based Metallic Glass"*, P. Ganesh and M. Widom, **Phys. Rev. B 77, 014205 (2008)**

21) *"Signature of Nearly Icosahedral Structures in Liquid and Supercooled Liquid Copper"*, P. Ganesh and M. Widom, **Phys. Rev. B 74, 134205 (2006)**

22) *"Empirical Oscillating Potentials for Alloys from ab initio Fits"*, M. Mihalkovic, C. L. Henley, M. Widom and P. Ganesh, **arXiv:0802.2926 (2008)**

ARTICLES TO BE SUBMITTED IN JANUARY 2013

1) *"Binding and Diffusion of Lithium in Graphite: Quantum Monte-Carlo benchmarks and validation of van der Waals density functional methods"*, P. Ganesh, Jeongnim Kim, Mina Yoon, P. R. C. Kent and Fernando Reboredo, **(to be submitted to Phys. Rev. Lett. (2012))**

2) *"Weak Lattice Interactions and Electronic Resonances in Epitaxially Grown Charge Transfer Salts"*, Geofferey A. Rojas, P. Ganesh, Simon Kelly, Bobby Sumpter, John Schlueter and Peter Maksymovich, **(to be submitted to Phys. Rev. Lett. (2012))**

ARTICLES IN PREPARATION

1) *"Reactive Force-Field Development for Supercapacitors and CO_2 Sequestration"*, P. Ganesh, L. Vlcek, Adri-van Duin and P. R. C. Kent.

2) *"Dynamic Properties of Ethylene Carbonate-Dimethyl Carbonate Electrolyte Mixtures for Li-ion Batteries from ab initio Molecular Dynamics"*, P. Ganesh, P. R. C. Kent and De-en Jiang

3) *"Pressure Induced Transitions in $PbTiO_3$ at Very High Pressures: Experiments and Theory"*, P. Ganesh, M. Ahart and R. E. Cohen

BOOK CHAPTER

1) *"Modeling Interactions of Metal Oxide Surfaces with Water in Chemical Sensors: Simulation and Modeling"*, L. Vlcek, P. Ganesh, A. Bandura, E. Mamantov, M. Predota, P. T. Cummings, D. J. Wesolowski, **Momentum Press, LLC (2012) (in press).**

AWARDS AND HONORS

2010 FIRST-EFRC Postdoctoral Fellowship
2007 Carnegie Institution of Washington Postdoctoral Fellowship
2006 The Joseph A. Kane Fellowship from the Physics Department, Carnegie Mellon University
2005 George E. and Majorie S. Pake Fellowship from the Mellon College of Science, Carnegie Mellon University
2000 Book award in physics, Department of Physics, University of Pune, India

GRANT WRITING EXPERIENCE

2013 Multiple successful CNMS user proposals to perform scientific reserch
2013 Co-PI on a US-DOE INCITE award of 45 million cpu hrs (PI: Dr. Paul R. C. Kent)
2011 Co-PI on a successful neutron proposal at LANSCE, Los Alamos (PI: Dr. Juergen Eckert)
2009 Significant contributor to a successful US-ONR grant proposal (PI: Dr. Ronald E. Cohen)

MEMBER OF SCIENTIFIC ORGANIZATIONS (Present and/or Past)

American Physical Society, American Chemical Society, Materials Research Society, Minerological Society of America