Panchapakesan Ganesh

FIRST-EFRC and NTI Postdoctoral Fellow
Center For Nanophase Materials Sciences Division
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Education

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

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

2010/7 –	FIRST-EFRC Fellow, Center for Nanophase Materials Sciences Division, ORNL
2007/7 – 2010/7	Postdoctoral Research Associate, Geophysical Laboratory, CIS
2006/7 – 2007/7	The Joseph A. Kane Research Fellow, Department of Physics, CMU
2005/9 – 2006/7	The George E. and Majorie S. Pake Fellow, Mellon College of Science, CMU
2002/9 – 2005/7	Research and Teaching Assistant, Department of Physics, CMU

Professional and Synergistic Activities

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

Honors and Awards

2010 –	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-ion batteries.*
   We use several methods 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-ion battery materials, in a wide range of length- and time-scales. The current focus is in understanding electrolytes and their interfaces with electrodes.
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 current focus in in understanding and quantifying the role of surface hydroxyls on reaction pathways and kinetics.

Previous Projects:

1. *Phase transitions in solids under pressure*
   We 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*
   We 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*
   We used *ab initio* molecular dynamics with statistical-mechanics to understand and predict the relation between geometric frustration and glass formability in metallic glasses.

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 Reviewd Publicaitons:
Over **180 citations** with an **h-index of 5**

1) *"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)**

2) *"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)**

3) *"Crystal structures of $(Mg_{1-x},Fe_x)SiO_3$ post-perovskite at high pressures"*, K. Hirose, W. Mao, Y. Meng, P. Ganesh, L. Shulenburger, G. Shen, Russell J. Hemley, **accepted in PNAS (January 5, 2012)**

4) *"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)**

5) *"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)**

6) *"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)**

7) *"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)**

8) *"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)**

9) *"First principles coexistence simulations of supercooled liquid silicon"*, P. Ganesh and M. Widom, **Journal of Noncrystalline Solids 357, 442 (2010)**

10) *"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")

11) *"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)

12) *"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)**

13) *"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)

14) *"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)**

15) *"Pressure induced phase transition in $PbTiO_3$"*, P. Ganesh and R. E. Cohen, **J. Phys: Condens. Matter 21, 064225 (2008)**

16) *"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)**

17) *"Signature of nearly icosahedral structures in liquid and supercooled liquid copper"***,** P. Ganesh and M. Widom, **Phys. Rev. B 74, 134205 (2006)**

18) *"Empirical oscillating potentials for alloys from ab initio fits"*, M. Mihalkovic, C. L. Henley, M. Widom and P. Ganesh, **arXiv:0802.2926 (2008)**

Articles Under Review :

1) *"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. Am. Chem. Soc. (2011)**

2) *"Solid-electrolyte interphase formations and electrolyte reduction at Li-ion battery carbon anodes: A first-principles molecular dynamics study"*, P. Ganesh, P. R. C. Kent and De-en Jiang, **submitted to J Phys. Chem. 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) *"Li-ion diffusion in graphite: A diffusion quantum monte-carlo benchmark study"*, P. Ganesh, Jeongnim Kim, P. R. C. Kent

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).**