Dr. Panchapakesan Ganesh

Senior Research & Development Staff Member
Group Leader, Nanomaterials Theory Institute Group
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 (CNMS = Center for Nanophase Materials Sciences; ORNL = Oak Ridge National Laboratory; CIS = Carnegie Institution for Science; CMU = Carnegie Mellon University)

2020 – PRESENT R&D Senior R&D Staff Member, Center for Nanophase Materials Sciences (CNMS) Division, Oak Ridge National Laboratory. Currently leading the Nanomaterials Theory Institute (NTI) Group. The NTI group provides and advances capabilities for theory and high performance simulation to enable fundamental understanding of physical and chemical properties of nanoscale materials.

2015 – 2020 R&D Staff Member, Oak Ridge National Laboratory. Leading theoretical research programs in multi-ferro-ionics, topological quantum-materials and electron-beam matter interactions, coupling advanced electronic-structure methods, high-throughput computing and data-analytics (ML/AI), to interpret novel experiments and support users at the Center for Nanophase Materials Sciences, ORNL

2012 – 2015 R&D Associate Research Staff, Oak Ridge National Laboratory. Lead research programs in multiferroics, energy materials and molecular self-assembly and support users at the 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

2021 MRS Spring-Meeting, Symposium Co-organizer on *Topological Quantum Materials*

2019– PRESENT Serving on the Proposal Review Board of the Center for Functional Nanomaterials at Brookhaven National Laboratory

2018 MRS Fall-Meeting Lead Organizer of Symposium titled: "*Harvesting Functional Defects in Energy Materials*"

2018 Led a Tutorial in MRS Fall-Meeting titled: "*Advances in Synchrotron X-Ray and Quantum Monte Carlo Techniques with Applications to Functional Materials*"

2017 MRS Fall-Meeting, Co-organizer of Symposium titled: "*Design, Control and Advanced Characterization of Functional Defects in Materials*"

2017 CNMS/SNS User Meeting Organizer for Workshop titled: "*Materials Informatics*"

2017 Co-chaired the theory session of the "*Quantum Matter Heterostructure"* SNS workshop

2015 Co-organizer of the International Workshop/Meeting that I brought to Knoxville/ORNL, titled: "*Fundamental Physics of Ferroelectrics and Related Materials (Ferro2015)"*

2014– PRESENT Serving on the Proposal Review Board of the Center for Nanophase Materials at Argonne National Laboratory

2011– PRESENT Chaired various symposium sessions in annual international APS and MRS meetings.
2011– PRESENT Invited reviewer for various DOE-BES proposals, LLNL computational grand-challenge proposals, ASCR-ALCC proposals, ORNL SEED/LDRD proposals
2006– PRESENT Active referee for top-tier ACS, APS, NPJ, IOP, and RSC Journals (~20 reviews/year)

Honors and Awards

2020	Division award for Distinguished Scientific Paper, ORNL
2020	Significant Event Award, ORNL
2017	Significant Event Award, ORNL
2016	Significant Event Award, ORNL
2013	Significant Event Award, ORNL
2010	FIRST-EFRC Fellowship, ORNL
2006	The Joseph A. Kane Research Fellow, Department of Physics, CMU
2005	The George E. and Majorie S. Pake Fellow, Mellon College of Science, CMU
2000	Book Award in Physics, Department of Physics, University of Pune, India

Mentoring Activities

Postdoctoral Trainees I advised: Nikhil Sivadas (ORNL), Anh Pham (ORNL), David Lingerfelt (ORNL), Guoxiang Hu (accepted a faculty position in CUNY), Janakiraman Balachandran (moved to Shell oil&energy as a Computational Research Scientist), Peter Doak (moved to CSED/ORNL as a Scientific Software Engineer), Lianshan Lin (absorbed at ORNL as Technical Staff), Houlong Zhuang (moved to a Faculty Position in Arizona State)
Doctoral Students I advised: Hakan Demir @ Georgia Tech (moved to a Postdoc position at the Univ. of Minnesota), Abhijit Dhakane @ ORNL/UT-Bredesen
Student Interns I advised in NTI-group: Andrew Lubimtsev (moved to a MS/PhD in comput. mater. at the Univ. of Tennessee), Jonathan Anchell (moved to SUNY-Buffalo for a PhD in physics), Helen Zhao (moved to industry as a computer scientist), Shreyas Muralidharan (moved to OSU to obtain his bachelors degree and now pursuing PhD at Stanford in electrical engineering), Jonathan Campbell (featured by ORISE), Lei Zhang (moved to a Postdoc position at CMU in comp. mats.), Abhijeet Dhakane (moved to pursue MS/PhD at the Univ. of Tennessee in data science), Anthony Yoshimura (moved to a Staff position at LLNL), John Hymel (moved to pursue a PhD at Georgia Tech.).

Successful Grants Led/Co-Led:

- (PI) Led an ORNL-LDRD proposal to design new quantum hybrid interfaces, titled: "*Hybrid Quantum Interfaces for Dissipationless Charge and Spin Conduction*". (~$0.98K)
- (Co-PI) Theory-lead on an ORNL-LDRD proposal to understand and design functional interfacial chemistry, titled: "*Operando 4D STEM to Probe Dynamic Chemical Reactivity: Integrated Approach to Understand and Design Functional Interfacial Chemistry*". (~$760K)
- (Co-PI) Theory-lead on an ORNL-LDRD proposal to build parallel data-analysis tools for materials informatics, titled: "*DAPPER: Data Analysis Parallel Package Maker - A Lego Set for Big Data Scientists*". (~$735K)
- (PI) Led an ORNL-LDRD proposal to understand and discover ionic conductivity in energy materials, titled: "*An Integrated Approach to the Design and Discovery of Fast Ionic Conducting Materials*". (~$1.13M)
- (Co-PI) Theory-lead on a SEED proposal to understand field-induced switching in molecular-ferroelectrics, titled: "*Structure and Modeling of Time Resolved Polarization Switching in Selected Organic Ferroelectrics*". (~$150K)
- (Co-PI) Theory-lead on an ORNL-LDRD proposal to understand ferroelectric switching in layered ferro-ionic materials, titled: "*Layered Ferroics by Design"*. (~$0.98M)
- (Co-PI) Theory-led ORNL-LDRD proposal to accelerate design and discovery of oxide heterostructures, titled: "*Accelerated Discovery and Design of Complex Materials"*. (~$545K)

- (Co-PI) Theory-lead on an ORNL-LDRD proposal to understand origin of Fe-based superconductivity, titled: "*Decoupling Structural and Electronic Variables in MBE-grown Films of Iron-based Superconductors*". (~$387K)
- (Co-PI) DOE Computational Materials Science award to establish a Quantum Monte Carlo (QMC) center at ORNL, named: "*Center for Predictive Simulation of Functional Materials*", (~$2M/yr for 4 yrs.; center renewal recently submitted around May 2020).

Successful Computational and Neutron Proposals Led/Co-Led:

- (PI) Competed for and renewed an annual ERCAP allocation at DOE's NERSC Supercomputing Center totaling ~10 Million Core Hours per year of compute-time for my research. Project title: "*Center for Predictive Simulation of Functional Materials*" (earlier title: *"Data Driven Discovery by Design of Functional Materials"*)
- (PI) Competed to win ~500 K Node-Hours of computing time on OLCF/SUMMIT via the ALCC award. Project title: "*Metastability in Driven Dynamical Systems for Next-Gen Microelectronics Applications*".
- (Co-PI) Competed to win ~180 K Node-Hours of computing time on OLCF/SUMMIT via the ALCC award. Project title: "*Electronic Structure and Excited States Dynamics of Quantum Materials*".
- (PI) Obtained ~13+ Million Core Hours of compute-time on OLCF-machines as a Director's Discretionary (DD) award to perform research on energy- & quantum-materials. Project title: "*Defects, Interfaces and Disorder in Correlated Quantum Materials*" (earlier title: "*Data Driven Discovery by Design of Energy Materials*")
- (Co-PI) Competed to win ~50 Million Cpu. Hrs on OLCF/TITAN via the INCITE award. Project title: "*Predictive and Insightful Calculations of Energy Materials*".
- (Co-PI) Competed to obtain neutron beam-time at the Spallation Neutron Sciences (SNS) via their User Program on several (~6+) proposals in the last 10 yrs., particularly on theory-driven projects where I have been the PI/Co-PI.

PATENTS

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

LIST OF INVITED TALKS AND PUBLICATIONS

MAJOR INVITED TALKS

2020 "*Functional Defects by Design in Energy and Quantum Materials",* MS&T20 Technical Meeting and Exhibition, Pittsburgh, PA

2020 "*Predicting Functional Defects by Design in Energy and Quantum Materials",* TMS2020 149th Annual Meeting and Exhibition, San Diego, CA

2019 *"Functional Defects by Design: A High-Throughput Approach to Energy Materials Discovery",* 236th ElectroChemical Society (ECS) Meeting, Atlanta, GA

2019 *"Predicting Functional Defects by Design in Energy and Quantum Materials"*, CNMS seminar series, Oak Ridge, TN

2018 *"Functional Defects by Design: A High- Throughput Approach to Energy Materials Discovery",* Conference on Electronic and Advanced Materials 2018, Orlando FL

2017 *"Functional Defects by Design: A High-Throughput Approach to Energy Materials Discovery"*, Department of Physics, Auburn University, Auburn, AL

2016 *"Elucidating the Role of Oxygen Vacancies, Cation Intermixing and Nanostructuring in Oxide Interfaces Using Theory and Computations"*, MRS Spring 2016 meeting at Phoenix, AZ

2016 *"Superionic Conductors: Role of Defects and Disorder on Sulfide and Oxide based Materials for Batteries and Fuel-Cells"*, 2016 Technical Conference between Hyundai Motor Company and Oak Ridge National Laboratory (postdoc acted as a proxy due to my personal travel)

2016 *"Superionic Conductors: Emerging Concepts and New Opportunities from Recent Computational Studies"*, Electrical Energy Storage (EES) lunch Seminar at ORNL, Oak Ridge, TN

2016 "*A High-Throughput Data Based Approach to Materials Discovery*", Workshop on Collective Phenomenon of 2D and Layered Materials, Oak Ridge, TN

2015 "*Searching for Simple Physical Truths in the Design of Complex Materials*", P. Ganesh, Department of Physics, Virginia Commonwealth University, Richmond, VA

2012 *"Towards a Larger Length/Timescale Simulation of Reactive Fluid-Solid Interfaces"*, Carnegie Institution for Science, Washington, DC

2011 *"Accurate Static and Dynamic Properties of Electrolytes for Li-ion Battery Applications"*, 242nd American Chemical Society (ACS) National Meeting, Denver, USA (Symposium organized by IBM)

2011 *"Origin of Diffuse Scattering in Relaxor Ferroelectrics"*, March Meeting of the American Physical Society (APS March Meeting), Dallas, USA

2010 *"Origin of Diffuse Scattering in Relaxor Ferroelectrics"*, 25th Anniversay of the international meeting titled: Advances in the Fundamental Physics of Ferroelectrics and Related Materials, Aspen Center for Physics, Aspen, USA

2009 *"Liquid-Liquid Transition in Supercooled Liquid Si"*, 6th International Discussion Meeting on Relaxations in Complex Systems (IDMRCS), Rome, Italy

PEER-REVIEWED PUBLICATIONS (ALSO VISIT MY GOOGLE SCHOLAR PAGE)

- Over **4000 citations** with **h-index of 30** and **!10-index of 53** with **14 papers each with ~100 citations**
- Publications in **Nature**, **Nature Materials, Nature Communications, PNAS**, **Phys. Rev. Lett., Nano Lett.** and **J. Phys. Chem. Lett.** journals, with **70+ publications as a CNMS-Staff.**
  (A '' indicates first-/last-/corresponding- authorship)*

1) *"Machine Learned Features from Density of States for Accurate Adsorption Energy Prediction",* Victor Fung, Guoxiang Hu, P. Ganesh and B. G. Sumpter, **Nature Communications, 12, 1 (2021)**

2) *"Work Function Engineering of 2D Materials: The Role of Polar Edge Reconstructions",* Guoxiang Hu, Victor Fung, Jingsong Huang and P. Ganesh*, **J. Phys. Chem. Lett., 12, 2320 (2021)**

3) *"Realizing Gapped Surface States in Magnetic Topological Insulator $MnBi_{2-x}Sb_xTe_4$",* Wonhee Ko, Marek Kolmer, Jiaqiang Yan, Anh D. Pham, Mingming Fu, Felix Lüpke, Satoshi Okamoto, Zheng Gai, **P. Ganesh**, An-Ping Li, arXiv:2003.00180 **(under review with Phys. Rev. Lett. in July 2020)**

4) *"Designing Magnetic Topological van der Waals Heterostructure",* Anh Pham and **P. Ganesh***, arXiv:2003.05840 **(under review with NPJ Comp. Mats. in July 2020)**

5) *"Piezoelectric Domain Walls in van der Waals Antiferroelectric $CuInP_2Se_6$"*, Andrius Dziaugys, Kyle Kelley, John A. Brehm, Lei Tao, Alexander Puretzky, Tianli Feng, Andrew O'Hara, Sabine Neumayer, Marius Chyasnavichyus, Eugene A. Eliseev, Juras Banys, Yulian Vysochanskii, Feng Ye, Bryan C. Chakoumakos, Michael A. Susner, Michael A. McGuire, Sergei V. Kalinin, **P. Ganesh**, Nina Balke, Sokrates T. Pantelides, Anna N. Morozovska and Petro Maksymovych, (**accepted in Nature Communications in July 2020**) [DOE/ORNL Highlight in preparation]

6) *"Tunable Quadruple-Well Ferroelectric van der Waals Crystals",* John A Brehm, Sabine M Neumayer, Lei Tao, Andrew O'Hara, Marius Chyasnavichus, Michael A Susner, Michael A McGuire, Sergei V Kalinin, Stephen Jesse, **P. Ganesh**, Sokrates T Pantelides, Petro Maksymovych, Nina Balke, **Nature Materials**, **19, 43 (2020)** [Work featured as an ORNL-News Highlight]

7) *"Predicting Synthesizable Multi-Functional Edge Reconstructions in Two-Dimensional Transition Metal Dichalcogenides"*, Guoxiang Hu, Victor Fung, Xiahan Sang, Raymond R. Unocic and **P. Ganesh***, **NPJ Comp. Mats., 6, 44 (2020)**

8) "*Doped NiO: The Mottness of a Charge Transfer Insulator*", Friedrike Wrobel, Hyowon Park, Changhee Sohn, Haw-Wen Hsiao, Jian-Min Zuo, Hyeondeok Shin, Ho Nyung Lee, **P. Ganesh**, Anouar Benali, Paul R. C. Kent, Olle Heinonen and Anand Bhattacharya, **Phys. Rev. B, 101, 195128 (2020)**

9) *"Doping a Bad Metal: Origin of Suppression of Metal-Insulator Transition in Non-Stoichiometric VO_2",* **P. Ganesh***, Frank Lechermann, Ilkka Kylanpaa, Jaron Krogel, Paul R. C. Kent, Olle Heinonen, **Phys. Rev. B, 101, 155129 (2020)** [ORNL/OLCF Highlight in preparation]

10) *"Quantum Material Topology via Defect Engineering",* Anh Pham and **P. Ganesh***, **Phys. Rev. B (Rapid), 100, 241110 (2020)**

11) *"Interfacial Stabilization for Epitaxial $CuCrO_2$ Delafossites",* Jong Mok Ok, Sangmoon Yoon, Andrew R. Lupini, **P. Ganesh**, Mathew F. Chisholm and Ho Nyung Lee, **NPJ Sci. Rep., 10, 11375 (2020)**

12) *"Understanding Beam-Induced Electronic Excitations in Materials"*, D. Lingerfelt, **P. Ganesh***, J. Jakowski and B. G. Sumpter, **J. Chem. Theory Comput., 16, 2 (2020)**

13) *"Thickness and Strain Dependence of Piezoelectric Coefficient in $BaTiO_3$ Thin Films"*, K. P. Kelley, D. E. Yilmaz, L. Collins, Y. Sharma, D. Akbarian, A.C.T. van Duin, **P. Ganesh***, R. K. Vasudevan, **Phys. Rev. M, 4, 024407 (2020)**

14) *"Superior Electrocatalytic Hydrogen Evolution at Engineered Non-Stoichiometric Two-Dimensional Transition Metal Dichalcogenide Edges",* Guoxiang Hu, Victor Fung, Xiahan Sang, Raymond R Unocic, **P Ganesh***, **J. Mater. Chem. A, 7, 18357 (2019)**

15) *"Electronically Nonadiabatic Structural Transformations Promoted by Electron Beams",* D. Lingerfelt, **P. Ganesh***, J. Jakowski and B. G. Sumpter, **Adv. Funct. Mater., 29, 1901901 (2019)**

16) *"Local structure of potassium doped nickel oxide: A combined experimental-theoretical study",* Friederike Wrobel, Hyeondeok Shin, George E. Sterbinsky, Haw-Wen Hsiao, Jian-Min Zuo, **P. Ganesh**, Jaron T. Krogel, Anouar Benali, Paul R. C. Kent, Olle Heinonen, and Anand Bhattacharya, **Phys. Rev. M, 3, 115003, (2019)**

17) *"Understanding the Influence of Defects and Surface Chemistry on Ferroelectric Switching: a ReaxFF Investigation of $BaTiO_3$"*, Dooman Akbarian, Dundar E. Yilmaz, Ye Cao, **P. Ganesh***, Ismaila Dabo, Jason Munro, Renee Van Ginhovan and Adri C. T. van Duin, **Physical Chemistry Chemical Physics, 21, 182401 (2019)**

18) *"Surface, Interface and Temperature Effects on the Phase Separation and Nano-Particle Self-Assembly of Bimetallic $Ni_{0.5}Ag_{0.5}$: A Molecular-Dynamics Study"*, Ryan H. Allaire, Abhijeet Dhakane, Reece Emery, **P. Ganesh**, Philip D. Rack, Lou Kondic, Linda Cummings and Miguel Fuentes-Cabrera, **Nanomaterials, 9, 1040 (2019)**

19) *"Multi-Modal Characterization Approach to Understand Proton Transport Mechanisms in Solid Oxide Fuel Cells"*, Raymond R Unocic, Jilai Ding, Janakiraman Balachandran, Xiahan Sang, Wei Guo, Jonathan D Poplawsky, Gabriel M Veith, Craig A Bridges, Nazanin Bassiri-Gharb, **P. Ganesh, Microscopy & Microanalysis, 25, 2048 (2019)**

20) *"A TD-DFT Treatment of Electronic Excitations in the STEM Spanning Dipole and Impact Scattering Regimes"*, David Lingerfelt, Jacek Jakowski, **P. Ganesh**, Bobby Sumpter, **Microscopy & Microanalysis, 25, 2300 (2019)**

21) *"Giant Negative Electrostriction and Dielectric Tunability in a van der Waals Layered Ferroelectric"*, Sabine M. Neumayer, Eugene A. Eliseev, Michael A. Susner, Alexander Tselev, Brian J. Rodriguez, John A. Brehm, Sokrates T. Pantelides, **P.Ganesh**, Stephen Jesse, Sergei V. Kalinin, Michael A. McGuire, Anna N. Morozovska, Petro Maksymovych, and Nina Balke, **Phys. Rev. M, 3, 024401 (2019)**

22) *"Dynamical Disparity Between Hydration Shell Water and RNA in a Hydrated RNA System"*, Debsindhu Bhowmik, **P. Ganesh**, Bobby G. Sumpter and Monojoy Goswami, **Phys. Rev. E, 98, 062407 (2018)**

23) *"Surface Reconstructions and Modified Surface States in $La_{1-x}Ca_xMnO_3$"*, Rama K. Vasudevan, Hemant Dixit, Alexander Tselev, Liang Qiao, Tricia Meyer, Valentino R. Cooper, Arthur P. Baddorf, Ho Nyung Lee, **P. Ganesh*** and Sergei V. Kalinin, **Phys. Rev. M, 2, 104418 (2018)**

24) *"The Influence of Local Distortions on Proton Mobility in Acceptor Doped Perovskites"*, Jilai Ding, Janakiraman Balachandran, Xiahan Sang, Wei Guo, Jonathan S. Anchell, Gabriel M. Veith, Craig A. Bridges, Yongqiang Cheng, Christopher M. Rouleau, Jonathan D. Poplawsky, Nazanin Bassiri-Gharb, Raymond R. Unocic and **P. Ganesh***, **Chemistry of Materials, 30, 4919 (2018)** [Work featured as a DOE Office of Science Highlight]

25) *"Nanoscale Control of Metal-Insulator Transition in Epitaxial Vanadium Dioxides"*, Y. Sharma, C. Sohn, J. Balachandran, Jaron T. Krogel, **P. Ganesh**, L. Collins, Q. Li, N. Balke, S. Kalinin, O. Heinonen, and H. N. Lee, **ACS Nano, 12, 7159 (2018)**

26) *"Oxygen Vacancy Formation Energies in $PbTiO_3/SrTiO_3$ Superlattice"*, Lipeng Zhang, Isaac Bredeson, P. R. C. Kent, Valentino R. Cooper, **P. Ganesh**, Haixuan Xu, **Phys. Rev. M, 2, 064409 (2018)**

27) *"Direct Atomic Fabrication and Dopant Positioning in Si using Electron Beams with Active Real Time Image-Based Feedback"*, S. Jesse, B.M. Hudak, E. Zarkadoula, J. Song, A. Maksov, M. Fuentes-Cabrera, **P. Ganesh**, I. Kravchenko, P.C. Snijders, A.R. Lupini, A. Borisevich, and S.V. Kalinin, **Nanotechnology, 29, 255303 (2018)**

28) *"Influence of Non-Stoichiometry on Proton Conductivity in Thin Film Yttrium-Doped Barium Zirconate"*, Jilai Ding, Janakiraman Balachandran, Xiahan Sang, Wei Guo, Jonathan S. Anchell, Gabriel M. Veith, Craig A. Bridges, Yongqiang Cheng, Christopher M. Rouleau, Jonathan D. Poplawsky, Nazanin Bassiri-Gharb, Raymond R. Unocic and **P. Ganesh***, **ACS Applied Materials and Interfaces, 10, 4816 (2018)**

29) *"Electronic Properties of Doped and Defective NiO: A Quantum Monte Carlo Study"*, H. Shin, Y. Luo, **P.Ganesh**, J. Balachandran, J. T. Krogel, P. R. C. Kent, A. Benali and O. Heinonen, **Phys. Rev. M, 1, 073603 (2017)**

30) *"Accuracy of Ab Initio Electron Correlation and Electron Densities in Vanadium Dioxide"*, Ilkka Kyl¨anp¨a, Janakiraman Balachandran, **P. Ganesh**, Olle Heinonen, Paul R. C. Kent, and Jaron T. Krogel, **Phys. Rev. M, 1, 065408 (2017)**

31) *"Defect Genome of Cubic Perovskites for Fuel Cell Applications"*, Janakiraman Balachandran, Lianshan Lin, Jonathan S. Anchell, Craig A. Bridges and **P. Ganesh***, **J Phys. Chem. C, 121, 26637 (2017)** [Work featured as a DOE Office of Science Highlight]

32) *"The Influence of the Local Structure on Proton Transport in a Solid Oxide Proton Conductor $La_{0.8}Ba_{1.2}GaO_{3.9}$"*, Yongqiang Cheng, Janakiraman Balachandran, Zhonghe Bi, Craig A. Bridges, Mariappan Parans Pranthaman, Luke L. Daemen, **P. Ganesh**, Niina Jalarvo, **Journal of Materials Chemisty A, 5, 15507 (2017)**

33) *"Metal Thio-and Selenophosphates as Multifunctional van der Waals Layered Materials"*, Michael A Susner, Marius Chyasnavichyus, Michael A McGuire, **P. Ganesh**, Petro Maksymovych, **Advanced Materials, 29, 1602852 (2017)**

34) *"Cation-Eutectic Transition via Sublattice Melting in $CuInP_2S_6/In_{4/3}P_2S_6$ van der Waals Layered Crystals"*, Michael A. Susner, Marius Chyasnavichyus, Alexander A. Puretzky, Qian He, Benjamin S. Conner, Yang Ren, David A. Cullen, Hakan Demir, **P. Ganesh**, Dongwon Shin, Jacob W. McMurray, Albina Y. Borisevich, Petro Maksymovich and Michael A. McGuire, **ACS Nano, 11, 7060 (2017)**

35) *"An Automated Analysis Workflow for Optimization of Force-Field Parameters using Neutron Scattering Data"*, V. E. Lynch, J. M. Borreguero, D. Bhowmik, **P. Ganesh**, B. G. Sumpter, T. E. Proffen and M. Goswami, **Journal of Computational Physics, 340, 128 (2017)**

36) *"Persistent Electrochemical Performance in Epitaxial VO_2"*, Shinbuhm Lee, Xiao-Guang Sun, Andrew A. Lubimtsev, Xiang Gao, **P. Ganesh**, Zac T. Ward, Gyula Eres, Mathew Chisholm, Sheng Dai, Ho Nyung Lee, **Nano Letters, 17, 2229 (2017)** [This work was an ORNL Story Tip, and garnered significant publicity from various news outlets]

37) *"Li-ion Site Disorder Driven Superionic Conductivity in Solid Electrolytes: A First-Principles Investigation of β-Li_3PS_4"*, Gopi Krishna Phani Dathar, Janakiraman Balachandran, Paul R. C. Kent, Adam J. Rondinone and **P. Ganesh***, **J. of Mat. Chem. A, 5, 1173, (2017)**

38) *"Enhanced Dynamics of Hydrated tRNA on Nanodiamond Surfaces: A Combined Neutron Scattering and MD Simulation Study"*, Gurpreet Dhindsa, Debsindhu Bhowmik, Monojoy Goswami, Hugh O'Neill, Eugene Mamontov, Bobby G. Sumpter, Liang Hong, **P. Ganesh*** and Xiang-chiang Chu, **J. Physical Chemistry B, 120, 10059 (2016)** [Work was featured as an ORNL Science Highlight, garnering significant publicity from various news outlets and the story was tweeted by the then NNSA Director]

39) *"Grain Boundary Stability and Influence on Ionic Conductivity in a Disordered Perovskite – a First-Principles Investigation of Lithium Lanthanum Titanate"*, Kathleen Alexander, **P. Ganesh***, Miaofang Chi, P. R. C. Kent and Bobby G. Sumpter, **MRS Communications, 6, 455, (2016)**

40) *"Thermodynamic Control of Two-Dimensional Molecular Ionic Nanostructures of TTF-TCNQ on Metal Surfaces"*, Seokmin Jeon, Peter Doak, Bobby G. Sumpter, **P. Ganesh** and Petro Maksymovich, **ACS Nano, 10, 7821 (2016)**

41) *"Tunable One-Dimensional Electron Gas Carrier Densities at Oxide Nanostructured Interfaces"*, Houlong L. Zhuang, L. Zhang, H. Xu, P. R. C. Kent, **P. Ganesh** and V. R. Cooper, **Sci. Rep., 6, 25352 (2016)**

42) *"Oxygen Vacancy Diffusion in Bulk $SrTiO_3$ from Density Functional Theory Calculations"*, Lipeng Zhang, Bin Liu, Houlong L. Zhuang, P. R. C. Kent, Valentino R. Cooper, **P. Ganesh** and Haixuan Xu, **Comp. Mats. Sci., 118, 309 (2016)**

43) *"Ultrathin Nanosheets of $CrSiTe_3$: a Semiconducting Two-dimensional Ferromagnetic Material"*, Ming-Wei Lin, Houlong L. Zhuang, Jiaqiang Yan, Thomas Zac Ward, Alexander A .Puretzky, Christopher M. Rouleau, Zheng Gai, Liangbo Liang, Vincent Meunier, Bobby G. Sumpter, **P. Ganesh**, Paul R. C. Kent, David B. Geohegan, David G. Mandrus and Kai Xiao, **J. Mat. Chem. C, 4, 315 (2016)**

44) *"Competitive Lithium Solvation of Linear and Cyclic Carbonates from Quantum Chemistry"*, Oleg Borodin, Marco Olguin, **P. Ganesh**, Paul R. C. Kent, Joshua L. Allen and Wesley A. Henderson, **Phys. Chem. Chem. Phys., 18, 164 (2016)**

45) *"High-T_c Layered Ferrielectric Crystals by Coherent Spinodal Decomposition"*, Michael A. Susner, Alex Belianinov, Albina Borisevich, Quan He, Marius Chyasnavichyus, Hakan Demir, David S. Sholl, **P. Ganesh**, Douglas L. Abernathy, Michael A. McGuire and Petro Maksymovich, **ACS Nano, 9, 12365 (2015)**

46) *"Benchmarking Density Functional Theory Predictions of Framework Structures and Properties in a Chemically Diverse Test Set of Metal Organic Frameworks"*, Dalar Nazarian, **P. Ganesh** and David S. Sholl, **J. Mats. Chem. A, 3, 22432 (2015)**

47) *"Plentiful Magnetic Moments in Oxygen Deficient $SrTiO_3$"*, Alejandro Lopez-Bezanilla, **P. Ganesh** and Peter B. Littlewood, **APL Materials, 3, 100701 (2015)**

48) *"Atomic Resolution Distortion Analysis of Yttrium-Doped Barium Zirconate"*, Jilai Ding, Xiahan Sang, Janakiraman Balachandran, Nazanin Bassiri-Gharb, **P. Ganesh** and Raymond R. Unocic, **Microscopy and Microanalysis, 22, 910-911 (2016)**

49) *"Rashba Effect in Single-Layer Antimony Telluroiodide SbTeI"*, Houlong L. Zhuang, Valentino R. Cooper, Haixuan Xu, **P. Ganesh**, Richard G. Hennig and P. R. C. Kent, **Phys. Rev. B, 92, 115302 (2015)**

50) *"Computational Discovery of Ferromagnetic Semiconducting Single-layer $CrSnTe_3$",* Houlong L. Zhuang, Yu Xie, P. R. C. Kent and **P. Ganesh***, **Phys. Rev. B, 92, 035407 (2015)**

51) *"A Reactive Force-Field Study of Li/C Systems for Electrical Energy Storage",* Muralikrishna Raju, **P. Ganesh***, P. R. C. Kent and Adri van Duin, **J. Chem. Theory Comput., 11, 2156 (2015)**

52) *"Surface Control of Epitaxial Manganite Films via Oxygen Pressure",* Alexander Tselev, Rama K. Vasudevan, Anthony G. Gianfrancesco, Liang Qiao, **P. Ganesh**, Tricia L. Meyer, Ho Nyung Lee, Michael D. Biegalski, Arthur P. Baddorf and Sergei V. Kalinin, **ACS Nano, 9, 4316 (2015)**

53) *"Role of Chalcogen Vapor Annealing in Inducing Bulk Superconductivity in $Fe_{(1+y)}Te_{(1-x)}Se_x$",* Wenzhi Lin, **P. Ganesh**, Anthony Gianfrancesco, Jun Wang, Tom Berlijn, Thomas A. Maier, Sergei V. Kalinin, Brian C. Sales and Minghu Pan, **Phys. Rev. B (R), 91, 060513 (2015)**

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