Dr. Panchapakesan Ganesh

Distinguished Research & Development Staff Member
Group Leader, Nanomaterials Theory Institute Group
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Education

Carnegie Mellon University, USA	Physics	Condensed Matter Theory	MS/PhD, 2007
University of Pune, Pune, India	Physics	Quantum Field Theory	MSc.,First-Class, 2002
Presidency College, Calcutta, India	Physics	with Honours	B.Sc., 2000

Professional Experience (CNMS = Center for Nanophase Materials Sciences; ORNL = Oak Ridge National Laboratory; CIS = Carnegie Institution for Science; CMU = Carnegie Mellon University;)

2024 – PRESENT	Distinguished R&D Staff Member and Group Leader of the Nanomaterials Theory Institute (NTI) group, Center for Nanophase Materials Sciences (CNMS) Division, Oak Ridge National Laboratory. The NTI group provides and advances capabilities for theory and high performance simulations to enable fundamental understanding of physical and chemical processes at the nanoscale, and support users at the Center for Nanophase Materials Sciences, ORNL.
2020 – 2024	Senior R&D Staff Member and Group Leader of the Nanomaterials Theory Institute (NTI) group, Center for Nanophase Materials Sciences (CNMS) Division, Oak Ridge National Laboratory.
2015 – 2020	R&D Staff Member, Oak Ridge National Laboratory. Leading research teams 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 improve understanding of nanoscale phase-transitions, interpret novel experiments at ORNL, and support users.
2012 – 2015	R&D Associate Research Staff Member, Oak Ridge National Laboratory. Lead research projects in multiferroics, energy materials and molecular self-assembly and support users.
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

2023	Initiated and Co-led the *TRANSIENT* workshop at ORNL bringing together national experts to understand the research status of out-of-equilibrium nanoscale processes
2022	MRS Fall-Meeting, Symposium Co-organizer for "*Harnessing Functional Defects for Energy and Electronic Frontiers*", Boston, MA
2022	MRS Spring-Meeting, Symposium Co-organizer for "*Harnessing Functional Defects in Energy and Electronic Materials*", Honolulu, Hawai'i
2021	Lead organizer of a 3-day international workshop titled: "*Artificial Intelligence in Multi-Fidelity, Multi-Scale and Multi-Physics Simulation of Materials*" as part of the Joint CNMS/SNS User Meeting.
2021	MRS Spring-Meeting, Lead Symposium Co-organizer on "*Predictive Synthesis and Decisive Characterization of Emerging Quantum Materials"*

2023– PRESENT Serving on the Chemistry, Geochemistry and Environmental Chemistry board of the Spallation Neutron Source (SNS).

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 and NSF proposals, LLNL computational grand-challenge proposals, ASCR-ALCC/INCITE 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: Soumendu Bagchi (ORNL), Abdulgani Annabardiyev (ORNL), Nikhil Sivadas (ORNL → Samsung R&D, Boston), Anh Pham (ORNL →Deloitte, Quantum Computing US Research Lead), David Lingerfelt (ORNL → ORNL Staff Member), Guoxiang Hu (ORNL → faculty in Georgia Tech), Victor Fung (ORNL → Faculty in Georgia Tech), Janakiraman Balachandran (ORNL → Computational Research Scientist at Shell Inc.), Peter Doak (ORNL → Senior Scientific Software Engineer at ORNL), Lianshan Lin (ORNL → Technical Staff at ORNL), Houlong Zhuang (ORNL → Faculty 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) **Leading** a proposal to develop a theoretical framework to achieve theory-guided discovery and autonomous synthesis of novel thin-film heterostructures for quantum applications, titled: "*Quantum Correlated Materials Accelerated Discovery Platform (Q-CAD)*" ($641K/yr for 3 years)
- (Co-PI) **Theory-lead** on an ORNL-SEED proposal titled: "*Chiral Materials for Next Generation Quantum Transduction*". ($190K)
- (Co-PI) **Theory-lead** on a 4 year DOE NSRC QIS infrastructure award titled: "*Precision Atomic Assemby for Quantum Information Sciences".* (~$7M)
- (PI) **Led** an ORNL-LDRD proposal to design new quantum hybrid interfaces, titled: "*Hybrid Quantum Interfaces for Dissipationless Charge and Spin Conduction*". (~$980K)
- (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 and **materials-thrust lead**) US 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 8 yrs.;).
- (Co-PI and **Group Leader**) *Center for Nanophase Materials Sciences*, US DOE user center at ORNL (~$25M/yr since 2012, US DOE scientific review for center renewal every ~3 years.)

In addition to this, I have advised several staff members over the last 10 years to successfully lead scientific proposals of their own, as well as advised several postdocs to find independent research/faculty positions.

Successful Computational and Neutron Proposals Led/Co-Led:

- (PI) DOE-INCITE proposal titled "*Exascale Ab Initio Simulations of Out-of-Equilibrium Heterogeneous Quantum Materials*" for ~175K Node hours on Frontier@OLCF.
- (Co-PI) Competed for and obtained ~1M Node-Hours of INCITE allocation on DOE's OLCF/ALCF exascale machines for project titled: "*Exascale Simulations of Quantum Materials*".
- (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

SELECTED INVITED TALKS

2024 "*Harnessing Electron Correlations and Anharmonicity for Energy Efficient Computing*", at the Electronic Materials and Applications (EMA) meeting, Denver, Colorado

2024 "*Understanding Phase Transitions in Correlated Quantum Materials*", at the Electronic Materials and Applications (EMA) meeting, Denver, Colorado

2023 "*Explaining Stabilization and Switching of Polarization in 2D Cu-thiophosphate Ferroelectrics*", March meeting of the American Physical Society (APS), Las Vegas, NV

2023 "*Understanding Phase Transitions in Correlated Quantum Materials*" at the 2nd Quantum Matters in Materials Science *(QMMS)* workshop, NIST, Gaithersburg, MD

2022 "*Harnessing Electron Correlations and Anharmonicity for Energy Efficient Computing*" at the Electronic Materials and Applications (EMA) meeting, Orlando, Florida

2022 "*Harnessing Electron Correlations and Anharmonicity for Energy Efficient Computing*" Nano4neuro international workshop, (Virtual)

2022 "*Harnessing Electron Correlations and Anharmonicity for Energy Efficient Computing*" Vanderbilt University, Nashville, Tennessee.

2021 "*Understanding Metal Insulator Transitions in Correlated Oxides for Rapid Electrical Switching*", US DOE CABLE Workshop, April 8th, 2021 (Virtual)

2020 "*Hybrid-Interfaces in Topological Quantum Materials*", On-Demand MRS Fall meeting talk, (Virtual)

2020 "*Excited State Pathways for Electron Beam Induced Point Defect Manipulation in Graphene Nanomaterials*", On-Demand MRS Fall meeting talk, (Virtual)

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"*, 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

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: 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*", International 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 **7200+ citations** with **h-index of 43** and **!10-index of 94** with **21 papers each with ~100+ citations**
- Publications in **Nature**, **Nature Materials, Nature Communications, PNAS**, **Phys. Rev. Lett., Nano Lett., Wiley Advanced Materials** and **J. Phys. Chem. Lett.** journals**.**

(A '' indicates first-/last-/corresponding- authorship)*

1) "*Enhanced Twist-Averaging Technique for Magnetic Metals: Applications Using Quantum Monte Carlo*", Abdulgani Annaberdiyev, **P. Ganesh**, Jaron T Krogel, **J. Chem. Theory Comput., 20, 2786 (2024)**

2) "*JARVIS-Leaderboard: a large scale benchmark of materials design methods*", Kamal Choudhary, Daniel Wines, Kangming Li, Kevin F Garrity, Vishu Gupta, Aldo H Romero, Jaron T Krogel, Kayahan Saritas, Addis Fuhr, **P. Ganesh**, Paul RC Kent, Keqiang Yan, Yuchao Lin, Shuiwang Ji, Ben Blaiszik, Patrick Reiser, Pascal Friederich, Ankit Agrawal, Pratyush Tiwary, Eric Beyerle, Peter Minch, Trevor David Rhone, Ichiro Takeuchi, Robert B Wexler, Arun Mannodi-Kanakkithodi, Elif Ertekin, Avanish Mishra, Nithin Mathew, Mitchell Wood, Andrew Dale Rohskopf, Jason Hattrick-Simpers, Shih-Han Wang, Luke EK Achenie, Hongliang Xin, Maureen Williams, Adam J Biacchi, Francesca Tavazza, **NPJ Computational Materials, 10, 93 (2024)**

3) "*DFT+U and Quantum Monte Carlo study of electronic and optical properties of $AgNiO_2$ and $AgNi_{1-x}Co_xO_2$ delafossite*", Hyeondeok Shin, **P. Ganesh**, Paul Kent, Anouar Benali, Anand Bhattacharya, Ho Nyung Lee, Olle Heinonen and Jaron Krogel, **Physical Chemistry Chemical Physics, 26, 6967 (2024)**

4) "*Bridging Theory with Experiment: Digital Twins and Deep Learning Segmentation of Defects in Monolayer MX_2 Phases*", Addis S Fuhr, **P. Ganesh**, Rama K Vasudevan, Bobby G Sumpter, **Applied Physics Letters**, **124, 031901 (2024)**

5) "*A First-Principles Study of Bilayer 1T'-WTe_2/CrI_3: A Candidate Topological Spin Filter*", Daniel Staros, Brenda Rubenstein and **P. Ganesh***, **NPJ Spintronics, 2, 4 (2024)**

6) "*Intermittent Defect Fluctuations in Oxide Heterostrucutres*", Q. Zhang, G. Wan, V. Starchenko, G. Hu, E.M. Dufresne, H. Zhou, H. Jeen, I. C. Almazan, Y. Dong, H. Liu, A. R. Sandy, G. E. Sterbinsky, Ho Nyung Lee, **P. Ganesh***, Dillon D. Fong, **Advanced Materials, 35, 2305383 (2023)**

7) "*Emergent Magnetism with Continuous Control in the Ultrahigh-Conductivity Layered Oxide $PdCoO_2$*", M. Brahlek, A. R. Mazza, A. Annaberdiyev, M. Chilcote, G. Rimal, G. B. Halasz, Anh Pham, Y. Pai, J. T. Krogel, J. Lapano, B. J. Lawrie, G. Eres, J. McChesney, T. Prokscha, A. Suter, S. Oh, J. W. Freeland, Y. Cao, J. S. Gardner, Z. Salman, R. G. Moore, **P. Ganesh***, T. Z. Ward, **Nano Letters, 23, 7279 (2023)**

8) "*Defects Go Green: Using Defects in Nanomaterials for Renewable Energy and Environmental Sustainability*", Addis S. Fuhr, Bobby G. Sumpter and P. Ganesh, **Frontiers in Nanotechnology, 5, (2023)**

9) "*The role of electron correlations in the electronic structure of putative Chern magnet $TbMn_6Sn_6$ using correlated methods*", Abdulgani Annaberdiyev, Lubos Mitas, Jaron T Krogel, **P. Ganesh***, **NPJ Quantum Materials, 8, 50 (2023)** [Submitted as a DOE Highlight]

10) "*Stacking Faults and Topological Properties in $MnBi_2Te_4$: Reconciling Gapped and Gapless States*", Jeonghwan Ahn, Seoung-Hun Kang, Mina Yoon, **P. Ganesh***, Jaron T Krogel, **J. Phys. Chem. Lett.**, **14, 9052 (2023)**

11) "*A Graph Dynamical neural network approach for decoding dynamical states in ferroelectrics*", A. Dhakane, T. Xie, D. E. Yilmaz, A. C. T. van Duin, B. G. Sumpter and **P. Ganesh***, **Carbon Trends, 11, 100264 (2023)**

12) "*Phase Transition Dynamics in a Complex Heterostructure*", Qingteng Zhang, Guoxiang Hu, Vitalii Starchenko, Gang Wan, Eric M Dufresne, Yongqi Dong, Huajun Liu, Hua Zhou, Hyoungjeen Jeen, Kayahan Saritas, Jaron T Krogel, Fernando A Reboredo, Ho Nyung Lee, Alec R Sandy, Irene Calvo Almazan, **P. Ganesh***, Dillon D Fong, **Phys. Rev. Lett., 129, 235701 (2023)** [Work featured as a news highlight]

13) "*The Atomic Drill Bit: Precision Controlled Atomic Fabrication of 2D Materials*", Matthew G Boebinger, Courtney Brea, Li-Ping Ding, Sudhajit Misra, Olugbenga Olunloyo, Yiling Yu, Kai Xiao, Andrew R Lupini, Feng Ding, Guoxiang Hu, **P. Ganesh**, Stephen Jesse, Raymond R Unocic, **Advanced Materials, 35, 2210116 (2023)**

14) "*Deterministic Conductive Filament Formation and Evolution for Improved Switching Uniformity in Embedded Metal-Oxide-Based Memristors─ A Phase-Field Study*", Kena Zhang, **P. Ganesh**, Ye Cao, **ACS Applied Materials & Interfaces, 15, 21219 (2023)**

15) "*Extraction of interaction parameters from specular neutron reflectivity in thin films of diblock copolymers: an inverse problem*", Dustin Eby, Mikolaj Jakowski, Valeria Lauter, Mathieu Doucet, **P. Ganesh***, Miguel Fuentes-Cabrera, Rajeev Kumar, **Nanoscale, 15, 7280 (2023)**

16) "*Atomic Structure Generation from Reconstructing Structural Fingerprints*", V. Fung, S. Jia, J. Zhang, S. Bi, J. Yin and **P. Ganesh***, **Machine Learning: S&T, 3, 045018 (2022)**

17) "*Role of Defects and Structure Evolution across Ferroelectric Phase Transitions Studied by Quantitative Aberration-Corrected STEM*", Albina Y Borisevich, Rama K Vasudevan, Kyle P Kelley, Sabine M Neumayer, Michael A Susner, Michael A McGuire, Anna N Morozovska, Eugene A Eliseev, **P. Ganesh**, Andrew O'Hara, Blair R Tuttle, Sokrates T Pantelides, Nina Balke, Peter Maksymovych, **Microscopy and Microanalysis, 28, 2360 (2022)**

18) "*Atomic-scale Fabrication of 1D-2D Nano Hetero-structures within 2D Materials through Automated Tracking and Electron Beam Control*", Matthew G Boebinger, Ayana Ghosh, Sudhajit Misra, Kevin Roccapriore, Kai Xiao, Andrew R Lupini, **P. Ganesh**, Maxim Ziatdinov, Sergei V Kalinin, Stephen Jesse, Raymond R Unocic, **Microscopy and Microanalysis, 28, 2178 (2022)**

19) "*Quantum Spin Hall Edge States and Interlayer Coupling in Twisted Bilayer WTe_2*", Felix Lüpke , Dacen Waters, Anh D. Pham, Jiaqiang Yan, David G. Mandrus, **P. Ganesh*** and Benjamin M. Hunt, **Nano Letters, 22, 14, 5674–5680 (2022)**

20) "*Physically Informed Machine Learning Prediction of Electronic Density of States*", V. Fung, **P. Ganesh** and B. G. Sumpter, **Chem. Mater., 34, 11, 4848–4855 (2022)**

21) "*Effect of electrode and oxide properties on the filament kinetics during electroforming in metal-oxide-based memories*", Kena Zhang, Yao Ren, **P. Ganesh**, Ye Cao, **NPJ Computational Materials, 8, 1, (2022)**

22) "*Origin of metal-insulator transitions in correlated perovskite metals*", M Chandler Bennett, Guoxiang Hu, Guangming Wang, Olle Heinonen, Paul RC Kent, Jaron T Krogel, **P. Ganesh***, **Physical Review Research Letters, 4, L022005 (2022)**

23) "*Reversible Hydrogen-Induced Phase Transformations in $La_{0.7}Sr_{0.3}MnO_3$ Thin Films Characterized by In Situ Neutron Reflectometry*", Alessandro R Mazza, Qiyang Lu, Guoxiang Hu, Haoxiang Li, James F Browning, Timothy R Charlton, Matthew Brahlek, **P. Ganesh**, Thomas Zac Ward, Ho Nyung Lee, Gyula Eres, **ACS Applied Materials and Interfaces, 14, 10898 (2022)**

24) "*Anharmonic Stabilization of Ferrielectricity in $CuInP_2Se_6$*", Nikhil Sivadas, Peter Doak and **P. Ganesh***, **Physical Review Research, 4, 013094 (2022)**

25) "*Understanding Heterogeneities in Quantum Materials*", Wonhee Ko, Zheng Gai, Alexander A. Puretzky, Liangbo Liang, Tom Berlijn, Jordan A. Hachtel, Kai Xiao, **P. Ganesh**, Mina Yoon, and An-Ping Li , **Advanced Materials, 2106909, (2022)**

26) "*Local manifestations of thickness-dependent topology and edge states in the topological magnet $MnBi_2Te_4$*", Felix Lüpke, Anh D. Pham, Yi-Fan Zhao, Ling-Jie Zhou, Wenchang Lu, Emil Briggs, Jerzy Bernholc, Marek Kolmer, Jacob Teeter, Wonhee Ko, Cui-Zu Chang, **P. Ganesh***, and An-Ping Li, **Phys. Rev. B, 105, 035423 (2022)**

27) "*A combined first principles study of the structural, magnetic, and phonon properties of monolayer CrI_3*", Daniel Staros, Guoxiang Hu, Juha Tiihonen, Ravindra Nanguneri, Jaron Krogel, M. Chandler Bennett, Olle Heinonen, **P. Ganesh***, and Brenda Rubenstein, **The Journal of Chemical Physics, 156, 014707 (2022)**

28) "*Quantum theory of electronic excitation and sputtering by transmission electron microscopy*", Anthony Yoshimura, Michael Lamparski, Joel Giedt, David Lingerfelt, Jacek Jakowski, **P. Ganesh**, Tao Yu, Bobby G Sumpter, Vincent Meunier, **Nanoscale, 10.1039/d2nr01018f (2022)**

29) "*From ground to excited electronic state dynamics of electron and ion irradiated graphene nanomaterials*", David Lingerfelt, **P. Ganesh***, Bobby G.Sumpter, Jacek Jakowski, **Theoretical and Computational Chemistry, 21, 87 (2022)**

30) "*Oxygen Vacancy Injection as a Pathway to Enhancing Electromechanical Response in Ferroelectrics*", Kyle P Kelley, Anna N Morozovska, Eugene A Eliseev, Vinit Sharma, Dundar E Yilmaz, Adri CT van Duin, **P. Ganesh**, Albina Borisevich, Stephen Jesse, Peter Maksymovych, Nina Balke, Sergei V Kalinin, Rama K Vasudevan, **Advanced Materials, 34, 2106426 (2022)**

31) "*Inverse Design of Two-Dimensional Materials with Invertible Neural Networks*", V. Fung, J. Zhang, G. Hu, **P. Ganesh** and B. G. Sumpter, **NPJ Computational Materials, 7, 1 (2021)**

32) *"Electron-Beam-Induced Molecular Plasmon Excitation and Energy Transfer in Silver Molecular Nanowires",* Tao Yu, David Lingerfelt, Jacek Jakowski, Mohammed A. Jabed, **P. Ganesh*** and Bobby G. Sumpter*,* **JPCA, 125, 74 (2021)**

33) *"Metal–insulator transition tuned by oxygen vacancy migration across TiO_2/VO_2 interface",* Qiyang Lu, C. Sohn, G. Hu, X. Gao, M. Chisholm, I. Kylanppaa, J. Krogel, P. Kent, O. Heinonen, **P. Ganesh** and H. N. Lee, **Scientific Reports, 10, 18554 (2020)**

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

35) *"Nonadiabatic Effects on Defect Diffusion in Silicon-Doped Nanographenes",* David Lingerfelt, Tao Yu, A. Yoshimura, **P. Ganesh***, J. Jakowski and Bobby. G. Sumpter, **NanoLetters, 21, 236 (2021)**

36) *"Twin-Domain Formation in Epitaxial Triangular Lattice Delafossites",* J. M. Ok, S. Yoon, A. R. Lupini, **P. Ganesh**, A. Huon, M. F. Chisholm and H. N. Lee, **ACS Appl. Mater. Interfaces, 13, 22059 (2021)**

37) *"Machine learned features from density of states for accurate adsorption energy prediction",* V. Fung, G. Hu, **P. Ganesh** and Bobby G. Sumpter, **Nature Communications, 12, 88 (2021)**

38) *"Strain-Induced Atomic-Scale Building Blocks for Ferromagnetism in Epitaxial $LaCoO_3$",* S. Yoon, X. Gao, J. M. Ok, Z. Liao, M-G. Han, Y. Zhu, **P. Ganesh**, M. F. Chisholm, W. S. Choi and H. N. Lee, **NanoLetters, 21, 4006 (2021)**

39) *"Designing Atomic Edge Structures in 2D Transition Metal Dichalcogenides for Improved Catalytic Activity",* Raymond Unocic, Xiahan Sang, Guoxiang Hu, Victor Fung, Matthew Boebinger, Kai Xiao, **P. Ganesh***,* **Microscopy & Microanalysis, 27, 964 (2021)**

40) *"High-throughput phase-field simulations and machine learning of resistive switching in resistive random-access memory",* K. Zhang, J. Wang, Y. Huang, L-Q. Chen, **P. Ganesh*** and Y. Cao, **NPJ Computational Materials, 6, 198 (2020)**

41) *"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, **Phys. Rev. B, 102, 115402 (2020)**

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

43) *"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]

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