

Aravind Krishnamoorthy

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Employment

- 2022–present **Assistant Professor**, *Texas A&M University*, College Station, USA
J. Mike Walker '66 Department of Mechanical Engineering
- 2016–2022 **Postdoctoral Research Associate**, *University of Southern California*, Los Angeles, USA
Collaboratory for Advanced Computing and Simulations
Supervisors: Prof. Priya Vashishta, Prof. Rajiv K. Kalia, Prof. Aiichiro Nakano

Education

- 2010–2016 **Ph.D, Materials Science**, *Massachusetts Institute of Technology*, Cambridge, USA
Thesis: Modeling Mechanisms of Growth and Breakdown of Iron Sulfides
Advisor: Prof. Bilge Yildiz
- 2006–2010 **B.Tech, Metallurgy and Materials Science**, *Indian Institute of Technology*, Chennai, India
Project: Phase Field Modeling of Polycrystalline Solidification
Advisor: Prof. Gandham Phanikumar

Research Experience

Faculty Research

- MATSAIL** ○ Investigating multiple phenomena including predictive manufacturing of materials, ultrafast far-from-equilibrium processes, and multiscale digital twins of material surfaces and interfaces

Postdoctoral Research

- Machine Learning** ○ Developed robust neural network quantum molecular dynamics models for potential energy surfaces of complex materials to investigate material structure and dynamics
○ Designed reinforcement learning scheme to discover synthesis schedule for quantum materials
○ Developed machine-learned models for real time analysis of ultrafast experimental data
○ Designed variational autoencoder to study structural phase transitions in MoWS₂ monolayer
- Computational Synthesis** ○ Elucidated multistage reaction pathways and atomic processes in CVD synthesis of MoS₂ using a ReaxFF forcefield I developed
○ Identified metastable phases during crystallization and growth of monolayer materials using large-scale reactive simulations
- Excited-state Dynamics** ○ Demonstrated control of non-equilibrium phonon distributions through anisotropic electron-phonon interactions
○ Identified facile pathway for semiconducting-metal phase transformation in 2D materials
○ Characterized ultrafast non-radiative energy decay in optically excited materials

Graduate Research

- Multiscale Modeling** ○ Developed a multiscale model to simulate corrosion passive film behavior by coupling atomic-scale processes (using DFT and kMC) to mesoscale microstructure (using phase-field)

Professional Activities and Service

- Symposium Organizer**
- Co-organized “Materials Genome Towards Exascale” in Spetses, Greece in June 2018
 - Co-organized “Machine Learning in Materials Genome” in Spetses, Greece in June 2019
 - Chaired “Emerging Trends in MD Simulations and Machine Learning” in APS Fall Meeting 2021
- Reviewer** I have reviewed papers submitted to Materials Science, Physics and Chemistry journals including *ACS Nano*, *Nanoscale*, *ACS Catalysis*, *Computer Physics Communications*, *ACS Applied Materials and Interfaces*, *Japanese Journal of Applied Physics*, *RSC Advances*, *Scientific Reports*, *Vacuum*, *Environmental Chemical Engineering*
- Member**
- American Physical Society
 - Materials Research Society

Publications

- [1] L. Yang, S. C. Tiwari, S. S. Jo, S. Hong, A. Mishra, **A. Krishnamoorthy**, R. K. Kalia, A. Nakano, R. Jaramillo, and P. Vashishta. “Unveiling oxidation mechanism of bulk ZrS_2 ”. *MRS Advances*, 6(11), 2021.
- [2] S. Hong, S. Tiwari, **A. Krishnamoorthy**, K.-i. Nomura, C. Sheng, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta. “Sulfurization of MoO_3 in the chemical vapor deposition synthesis of MoS_2 enhanced by an H_2S/H_2 mixture”. *The Journal of Physical Chemistry Letters*, 12(7):1997–2003, 2021.
- [3] P. Rajak, N. Baradwaj, K.-i. Nomura, **A. Krishnamoorthy**, J. P. Rino, K. Shimamura, S. Fukushima, F. Shimojo, R. Kalia, A. Nakano, and P. Vashishta. “Neural network quantum molecular dynamics, intermediate range order in $GeSe_2$, and neutron scattering experiments”. *The Journal of Physical Chemistry Letters*, 12(25):6020–6028, 2021.
- [4] **A. Krishnamoorthy**, N. Baradwaj, A. Nakano, R. K. Kalia, and P. Vashishta. “Lattice thermal transport in two-dimensional alloys and fractal heterostructures”. *Scientific Reports*, 11(1), 2021.
- [5] **A. Krishnamoorthy**, A. Mishra, D. Kamal, S. Hong, K. ichi Nomura, S. Tiwari, A. Nakano, R. Kalia, R. Ramprasad, and P. Vashishta. “EZFF: Python library for multi-objective parameterization and uncertainty quantification of interatomic forcefields for molecular dynamics”. *SoftwareX*, 13:100663, 2021.
- [6] **A. Krishnamoorthy**, S. C. Tiwari, A. Nakano, R. K. Kalia, and P. Vashishta. “Electric-field-induced crossover of polarization reversal mechanisms in $Al_{1-x}Sc_xN$ ferroelectrics”. *Nanotechnology*, 32(49):49LT02, 2021.
- [7] **A. Krishnamoorthy**, K.-i. Nomura, N. Baradwaj, K. Shimamura, P. Rajak, A. Mishra, S. Fukushima, F. Shimojo, R. Kalia, A. Nakano, and P. Vashishta. “Dielectric constant of liquid water determined with neural network quantum molecular dynamics”. *Phys. Rev. Lett.*, 126:216403, 2021. (**Editor’s Choice**).
- [8] A. Britz, A. R. Attar, X. Zhang, H.-T. Chang, C. Nyby, **A. Krishnamoorthy**, S. H. Park, S. Kwon, M. Kim, D. Nordlund, S. Sainio, T. F. Heinz, S. R. Leone, A. M. Lindenberg, A. Nakano, P. Ajayan, P. Vashishta, D. Fritz, M.-F. Lin, and U. Bergmann. “Carrier-specific

dynamics in 2H-MoTe₂ observed by femtosecond soft x-ray absorption spectroscopy using an x-ray free-electron laser”. *Structural Dynamics*, 8(1):014501, 2021.

- [9] P. Rajak, **A. Krishnamoorthy**, A. Mishra, R. Kalia, A. Nakano, and P. Vashishta. “Autonomous reinforcement learning agent for chemical vapor deposition synthesis of quantum materials”. *npj Computational Materials*, 7(1), 2021.
- [10] L. Bassman, K. Liu, **A. Krishnamoorthy**, T. Linker, Y. Geng, D. Shebib, S. Fukushima, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta. “Towards simulation of the dynamics of materials on quantum computers”. *Phys. Rev. B*, 101:184305, 2020.
- [11] C. Shen, Y. Liu, J. Wu, C. Xu, D. Cui, Z. Li, Q. Liu, Y. Li, Y. Wang, X. Cao, H. Kumazoe, F. Shimojo, **A. Krishnamoorthy**, R. K. Kalia, A. Nakano, P. D. Vashishta, M. R. Amer, A. N. Abbas, H. Wang, W. Wu, and C. Zhou. “Tellurene photodetector with high gain and wide bandwidth”. *ACS Nano*, 14(1):303–310, 2020.
- [12] A. R. Attar, H.-T. Chang, A. Britz, X. Zhang, M.-F. Lin, **A. Krishnamoorthy**, T. Linker, D. Fritz, D. M. Neumark, R. K. Kalia, A. Nakano, P. Ajayan, P. Vashishta, U. Bergmann, and S. R. Leone. “Simultaneous observation of carrier-specific redistribution and coherent lattice dynamics in 2H-MoTe₂ with femtosecond core-level spectroscopy”. *ACS Nano*, 14(11):15829–15840, 2020.
- [13] **A. Krishnamoorthy**, P. Rajak, S. Hong, K. ichi Nomura, S. Tiwari, R. K. Kalia, A. Nakano, and P. Vashishta. “Reactive molecular dynamics simulations and machine learning”. *Journal of Physics: Conference Series*, 1461:012182, 2020.
- [14] S. Tiwari, **A. Krishnamoorthy**, P. Rajak, P. Sakdhnagool, M. Kunaseth, F. Shimojo, S. Fukushima, A. Nakano, Y. Luo, R. Kalia, K.-I. Nomura, and P. Vashishta. “Quantum dynamics at scale: Ultrafast control of emergent functional materials”. *Proceedings of HPC Asia 2020*, 2020. (**Best Paper Finalist**).
- [15] T. Linker, S. Tiwari, S. Fukushima, R. K. Kalia, **A. Krishnamoorthy**, A. Nakano, K.-i. Nomura, K. Shimamura, F. Shimojo, and P. Vashishta. “Optically induced three-stage picosecond amorphization in low-temperature SrTiO₃”. *The Journal of Physical Chemistry Letters*, 11(22):9605–9612, 2020.
- [16] P. Rajak, K. Liu, **A. Krishnamoorthy**, R. K. Kalia, A. Nakano, K.-i. Nomura, S. C. Tiwari, and P. Vashishta. “Neural network molecular dynamics at scale”. pages 991–994, 2020.
- [17] H. Yang, B. Chen, B. Song, D. Meng, S. Tiwari, **A. Krishnamoorthy**, X. Yan, Z. Liu, Y. Wang, P. Hu, T.-H. Ou, P. Branicio, R. Kalia, A. Nakano, P. Vashishta, F. Liu, H. Wang, and W. Wu. “Memristive device characteristics engineering by controlling the crystallinity of switching layer materials”. *ACS Applied Electronic Materials*, 2(6):1529–1537, 2020.
- [18] S. S. Jo, A. Singh, L. Yang, S. C. Tiwari, S. Hong, **A. Krishnamoorthy**, M. G. Sales, S. M. Oliver, J. Fox, R. L. Cavaleiro, D. W. Snyder, P. M. Vora, S. J. McDonnell, P. Vashishta, R. K. Kalia, A. Nakano, and R. Jaramillo. “Growth kinetics and atomistic mechanisms of native oxidation of ZrS_xSe_{2-x} and MoS₂ crystals”. *Nano Letters*, 20(12):8592–8599, 2020.
- [19] **A. Krishnamoorthy**, A. Mishra, N. Grabar, N. Baradwaj, R. K. Kalia, A. Nakano, and P. Vashishta. “Evolutionary multi-objective optimization and Pareto-frontal uncertainty quantification of interatomic forcefields for thermal conductivity simulations”. *Computer Physics Communications*, 254:107337, 2020.

- [20] A. Apte, **A. Krishnamoorthy**, J. A. Hachtel, S. Susarla, J. Yoon, L. M. Sassi, P. Bharadwaj, J. M. Tour, J. C. Idrobo, R. K. Kalia, A. Nakano, P. Vashishta, C. S. Tiwary, and P. M. Ajayan. "Two-dimensional lateral epitaxy of 2H (MoSe₂) - 1T' (ReSe₂) phases". *Nano Letters*, 19(9):6338–6345, 2019.
- [21] **A. Krishnamoorthy**, P. Rajak, P. Norouzzadeh, D. J. Singh, R. K. Kalia, A. Nakano, and P. Vashishta. "Thermal conductivity of MoS₂ monolayers from molecular dynamics simulations". *AIP Advances*, 9(3):035042, 2019.
- [22] P. Rajak, **A. Krishnamoorthy**, A. Nakano, P. Vashishta, and R. Kalia. "Structural phase transitions in a MoWSe₂ monolayer: Molecular dynamics simulations and variational autoencoder analysis". *Physical Review B*, 100(1):014108, 2019.
- [23] A. Apte, E. Bianco, **A. Krishnamoorthy**, S. Yazdi, R. Rao, N. Glavin, H. Kumazoe, V. Varshney, A. Roy, F. Shimojo, E. Ringe, R. K. Kalia, A. Nakano, C. S. Tiwari, P. Vashishta, V. Kochat, and P. M. Ajayan. "Polytypism in ultrathin tellurium". *2D Materials*, 6(1):9, 2019.
- [24] L. Q. Li, M. F. Lin, X. Zhang, A. Britz, **A. Krishnamoorthy**, R. R. Ma, R. K. Kalia, A. Nakano, P. Vashishta, P. Ajayan, M. C. Hoffmann, D. M. Fritz, U. Bergmann, and O. V. Prezhdo. "Phonon-suppressed auger scattering of charge carriers in defective two-dimensional transition metal dichalcogenides". *Nano Letters*, 19(9):6078–6086, 2019.
- [25] **A. Krishnamoorthy**, M. F. Lin, X. Zhang, C. Weninger, R. R. Ma, A. Britz, C. S. Tiwary, V. Kochat, A. Apte, J. Yang, S. Park, R. K. Li, X. Z. Shen, X. J. Wang, R. Kalia, A. Nakano, F. Shimojo, D. Fritz, U. Bergmann, P. Ajayan, and P. Vashishta. "Optical control of non-equilibrium phonon dynamics". *Nano Letters*, 19(8):4981–4989, 2019.
- [26] S. Hong, K. Nomura, **A. Krishnamoorthy**, P. Rajak, C. Y. Sheng, R. K. Kalia, A. Nakano, and P. Vashishta. "Defect healing in layered materials: A machine learning-assisted characterization of MoS₂ crystal phases". *Journal of Physical Chemistry Letters*, 10(11):2739–2744, 2019.
- [27] I. C. Tung, **A. Krishnamoorthy**, S. Sadasivam, H. Zhou, Q. Zhang, K. L. Seyler, G. Clark, E. M. Mannebach, C. Nyby, F. Ernst, D. Zhu, J. M. Glowina, M. E. Kozina, S. Song, S. Nelson, H. Kumazoe, F. Shimojo, R. K. Kalia, P. Vashishta, P. Darancet, T. F. Heinz, A. Nakano, X. Xu, A. M. Lindenberg, and H. Wen. "Anisotropic structural dynamics of monolayer crystals revealed by femtosecond surface X-ray scattering". *Nature Photonics*, 13(6):425, 2019.
- [28] A. Apte, **A. Krishnamoorthy**, J. A. Hachtel, S. Susarla, J. C. Idrobo, A. Nakano, R. K. Kalia, P. Vashishta, C. S. Tiwary, and P. M. Ajayan. "Telluride-based atomically thin layers of ternary two-dimensional transition metal dichalcogenide alloys". *Chemistry of Materials*, 30(20):7262–7268, 2018.
- [29] A. Apte, V. Kochat, P. Rajak, **A. Krishnamoorthy**, P. Manimunda, J. A. Hachtel, J. C. Idrobo, S. A. Syed Amanulla, P. Vashishta, A. Nakano, R. K. Kalia, C. S. Tiwary, and P. M. Ajayan. "Structural phase transformation in strained monolayer MoWSe₂ alloy". *ACS Nano*, 12(4):3468–3476, 2018.
- [30] K. Liu, S. Tiwari, C. Sheng, **A. Krishnamoorthy**, S. Hong, P. Rajak, R. K. Kalia, A. Nakano, K. Nomura, P. Vashishta, M. Kunaseth, S. Naserifar, W. A. Goddard, Y. Luo, N. A. Romero, and F. Shimojo. "Shift-collapse acceleration of generalized polarizable reactive molecular dynamics for machine learning-assisted computational synthesis of layered materials". *Scala 2018*:

- [31] **A. Krishnamoorthy**, L. Bassman, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta. “Semiconductor-metal structural phase transformation in MoTe₂ monolayers by electronic excitation”. *Nanoscale*, 10(6):2742–2747, 2018. (**Journal Cover Article**).
- [32] C. Sheng, S. Hong, **A. Krishnamoorthy**, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta. “Role of H transfer in the gas-phase sulfidation process of MoO₃: A quantum molecular dynamics study”. *Journal of Physical Chemistry Letters*, 9(22):6517–6523, 2018.
- [33] H. Kumazoe, **A. Krishnamoorthy**, L. Bassman, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta. “Photo-induced lattice contraction in layered materials”. *Journal of Physics-Condensed Matter*, 30(32):32LT02, 2018.
- [34] **A. Krishnamoorthy**, L. Bassman, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta. “Kinetics and atomic mechanisms of structural phase transformations in photoexcited monolayer TMDCs”. *MRS Advances*, 3(6-7):1–6, 2018.
- [35] A. Mishra, **A. Krishnamoorthy**, P. Rajak, S. Tiwari, C. Sheng, R. K. Kalia, A. Nakano, and P. Vashishta. “Free energy of hydration and heat capacity of calcium dipicolinate in *Bacillus* spore cores”. *Applied Physics Letters*, 113(11):113702, 2018.
- [36] L. Bassman, **A. Krishnamoorthy**, H. Kumazoe, M. Misawa, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta. “Electronic origin of optically-induced sub-picosecond lattice dynamics in MoSe₂ monolayer”. *Nano Letters*, 18(8):4653–4658, 2018.
- [37] S. Hong, C. Sheng, **A. Krishnamoorthy**, P. Rajak, S. Tiwari, K.-i. Nomura, M. Misawa, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta. “Chemical vapor deposition synthesis of MoS₂ layers from the direct sulfidation of MoO₃ surfaces using reactive molecular dynamics simulations”. *The Journal of Physical Chemistry C*, 122(13):7494–7503, 2018.
- [38] M.-F. Lin, V. Kochat, **A. Krishnamoorthy**, L. Bassman, C. Weninger, Q. Zheng, X. Zhang, A. Apte, C. S. Tiwary, X. Shen, R. Li, R. Kalia, P. Ajayan, A. Nakano, P. Vashishta, F. Shimojo, X. Wang, D. M. Fritz, and U. Bergmann. “Ultrafast non-radiative dynamics of atomically thin MoSe₂”. *Nature Communications*, 8(1):1745, 2017. (**News articles in Phys.org and SLAC News**).
- [39] M. Misawa, S. Tiwari, S. Hong, **A. Krishnamoorthy**, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta. “Reactivity of sulfur molecules on MoO₃ (010) surface”. *Journal of Physical Chemistry Letters*, 8(24):6206–6210, 2017.
- [40] V. Kochat, A. Apte, J. A. Hachtel, H. Kumazoe, **A. Krishnamoorthy**, S. Susarla, J. C. Idrobo, F. Shimojo, P. Vashishta, R. Kalia, A. Nakano, C. S. Tiwary, and P. M. Ajayan. “Re doping in 2D transition metal dichalcogenides as a new route to tailor structural phases and induced magnetism”. *Advanced Materials*, 29(43):1703754, 2017. (**Journal Cover Article**).
- [41] **A. Krishnamoorthy**, M. A. Dinh, and B. Yildiz. “Hydrogen weakens interlayer bonding in layered transition metal sulfide Fe_{1+x}S”. *Journal of Materials Chemistry A*, 5(10):5030, 2017.
- [42] P. Rajak, A. Mishra, C. Y. Sheng, S. Tiwari, **A. Krishnamoorthy**, R. K. Kalia, A. Nakano, and P. Vashishta. “Gel phase in hydrated calcium dipicolinate”. *Applied Physics Letters*, 111(21):213701, 2017. (**Journal Cover Article**).

- [43] S. Hong, **A. Krishnamoorthy**, P. Rajak, S. Tiwari, M. Misawa, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta. “Computational synthesis of MoS₂ layers by reactive molecular dynamics simulations: Initial sulfidation of MoO₃ surfaces”. *Nano Letters*, 17(8):4866–4872, 2017.
- [44] **A. Krishnamoorthy** and B. Yildiz. “Quantifying the origin of inter-adsorbate interactions on reactive surfaces for catalyst screening and design”. *Physical Chemistry Chemical Physics*, 17(34):22227–22234, 2015.
- [45] F. William Herbert, **A. Krishnamoorthy**, L. Rands, K. J. Van Vliet, and B. Yildiz. “Magnetic diffusion anomaly at the Néel temperature of pyrrhotite, Fe_{1-x}S”. *Physical Chemistry Chemical Physics*, 17(16):11036–11041, 2015.
- [46] F. W. Herbert, **A. Krishnamoorthy**, B. Yildiz, and K. J. Van Vliet. “Diffusion-limited kinetics of the antiferromagnetic to ferrimagnetic λ -transition in Fe_{1-x}S”. *Applied Physics Letters*, 106(9):092402, 2015.
- [47] F. W. Herbert, **A. Krishnamoorthy**, W. Ma, K. J. Van Vliet, and B. Yildiz. “Dynamics of point defect formation, clustering and pit initiation on the pyrite surface”. *Electrochimica Acta*, 127:416–426, 2014.
- [48] F. W. Herbert, **A. Krishnamoorthy**, K. J. Van Vliet, and B. Yildiz. “Quantification of electronic band gap and surface states on FeS₂(100)”. *Surface Science*, 618:53–61, 2013. (**News article in MIT News**).
- [49] **A. Krishnamoorthy**, F. W. Herbert, S. Yip, K. J. Van Vliet, and B. Yildiz. “Electronic states of intrinsic surface and bulk vacancies in FeS₂”. *Journal of Physics: Condensed Matter*, 25(4):045004–045004, 2013.

Papers under review

- [50] C. Tiwary, A. K. Singh, P. Kumbhakar, **A. Krishnamoorthy**, A. Nakano, K. K. Sadasivuni, P. Vashishta, A. K. Roy, and V. Kochat. “Strategies towards development of alloy two-dimensional transitional metal di-chalcogenides: Summary and Perspective”. *iScience*, 2021.
- [51] L. M. Sassi, **A. Krishnamoorthy**, J. A. Hachtel, S. Susarla, A. Apte, S. Castro, R. Vajtai, J. C. Idrobo, A. B. Puthirath, P. Vashishta, C. S. Tiwary, , and P. M. Ajayan. “Low temperature growth of WSe₂ by moisture-assisted defects in the precursor WO₃ powder”. *ACS Nano*, 2021.
- [52] A. B. Puthirath, X. Zhang, **A. Krishnamoorthy**, F. S. Samghabadi, D. C. Moore, J. Lai, T. Zhang, D. E. Sanchez, F. Zhang, R. Xu, N. R. Glavin, D. Litvinov, R. Vajtai, V. Swaminathan, M. Terrones, H. Zhu, P. Vashishta, and P. M. Ajayan. “Amplified piezoelectricity at metal semiconductor 2D interfaces in MoTe₂”. *Science*, 2021.

Papers in preparation

- [53] **A. Krishnamoorthy**, L. Yang, R. Kalia, A. Nakano, and P. Vashishta. “Thermal conductivity of strained and buckled two-dimensional materials”. *Under preparation*.
- [54] **A. Krishnamoorthy**, P. Rajak, A. Nakano, R. Kalia, and P. Vashishta. “Quantum molecular dynamics using machine learning augmented empirical forcefields”. *Under preparation*.
- [55] **A. Krishnamoorthy**, A. Nakano, R. Kalia, and P. Vashishta. “Machine learning (ML) for ultrafast electron diffraction (UED)”. *Under preparation*.

- [56] **A. Krishnamoorthy**, P. Rajak, A. Nakano, R. Kalia, and P. Vashishta. "Curl-corrected direct force prediction for robust machine-learned molecular dynamics simulations". *Under preparation*.

Invited Talks

- Virginia 2021** **Aravind Krishnamoorthy**, "Machine learning for material properties and design", in *Condensed Matter Physics Symposium, Department of Physics, University of Virginia*, (Charlottesville, VA, USA), 2021.
- Boston 2019** **Aravind Krishnamoorthy**, "Machine learning for ultrafast electron diffraction", in *American Physical Society March Meeting 2019*, (Boston, MA, USA), 2019.
- Spetses 2018** **Aravind Krishnamoorthy**, "Insights from simulations and experiments at similar length and time-scales", in *Spetses Symposium on Machine Learning at Exascale*, (Spetses, Greece), 2018.
- Kumamoto 2017** **Aravind Krishnamoorthy**, Lindsay Bassman, Aiichiro Nakano, Rajiv Kalia, Priya Vashishta, and Fuyuki Shimojo, "Atomic dynamics and structural phase transformations in optically excited 2D materials", in *5th International Symposium on Kumamoto Synchrotron Radiation*, (Kumamoto, Japan), 2017.

Contributed Conference Presentations

- APS 2021** **Aravind Krishnamoorthy**, Subodh Tiwari, Aiichiro Nakano, Rajiv Kalia, and Priya Vashishta, "Mechanism of reversible field-driven switching in ultra-high-polarization $\text{Al}_{1-x}\text{Sc}_x\text{N}$ ", in *APS March Meeting*, (Online), American Physical Society, 2021. (**Symposium Organizer**).
- MRS 2019** **Aravind Krishnamoorthy**, "Machine learning of reaction pathways in chemical vapor deposition for directed synthesis of two-dimensional chalcogenides", in *MRS Fall Meeting*, (Boston, MA), Materials Research Society, 2019.
- APS 2019** **Aravind Krishnamoorthy**, Pankaj Rajak, Sungwook Hong, Aiichiro Nakano, Rajiv Kalia, and Priya Vashishta, "Machine learning of reaction pathways in chemical vapor deposition of MoS_2 monolayers", in *APS March Meeting*, (Boston, MA), American Physical Society, 2019.
- APS 2017** **Aravind Krishnamoorthy**, Lindsay Bassman, Rajiv Kalia, Aiichiro Nakano, Fuyuki Shimojo, and Priya Vashishta, "Exploring ultrafast dynamics in photoexcited layered materials by large-scale quantum molecular dynamics simulations", in *APS March Meeting*, (New Orleans, LA), American Physical Society, 2017.
- Aravind Krishnamoorthy**, Lindsay Bassman, Rajiv Kalia, Aiichiro Nakano, Fuyuki Shimojo, and Priya Vashishta, "Kinetics and atomic mechanisms of rapid semiconductor-to-metal transitions in monolayer TMDs", in *APS March Meeting*, (New Orleans, LA), American Physical Society, 2017.
- MRS 2015** **Aravind Krishnamoorthy** and Bilge Yildiz, "*Ab initio* modeling of electrochemical reactions at the semiconductor-water interface", in *MRS Fall Meeting*, (Boston, MA), Materials Research Society, 2015.
- Aravind Krishnamoorthy**, Minh A. Dinh, and Bilge Yildiz, "Hydrogen point defects weaken interlayer bonding in layered transition metal sulfide, mackinawite Fe_{1+x}S ", in *MRS Fall Meeting*, (Boston, MA), Materials Research Society, 2015.
- Aravind Krishnamoorthy** and Bilge Yildiz, "Effect of local magnetic order on cationic mobility in iron sulfide, Fe_{1-x}S ", in *MRS Fall Meeting*, (Boston, MA), Materials Research Society, 2015.
- TMS 2014** **Aravind Krishnamoorthy**, William F. Herbert, and Bilge Yildiz, "Effect of Vacancy Ordering and Order-Disorder Transitions on Ionic Diffusivity in Iron-Sulfide Passive Corrosion Films",

in *143rd TMS Annual Meeting*, (San Diego, CA), The Minerals, Metals & Materials Society, 2014.

- MRS 2014 Aravind Krishnamoorthy**, William F. Herbert, and Bilge Yildiz, "Growth and breakdown of iron sulfide passive corrosion films – Towards a mechanistic, multiscale model", in *MRS Fall Meeting*, (Boston, MA), Materials Research Society, 2014.
- MMM 2014 Aravind Krishnamoorthy**, William F. Herbert, and Bilge Yildiz, "Growth and breakdown of iron sulfide passive corrosion films – Towards a mechanistic, multiscale model", in *7th International Conference on Multiscale Materials Modeling*, (Berkeley, CA), Institute of Physics, 2014.
- MRS 2013 Aravind Krishnamoorthy**, Minh A. Dinh, and Bilge Yildiz, "Hydrogen-induced delamination of mackinawite (Fe_{1+x}S) surface films in corrosive environments", in *MRS Fall Meeting*, (Boston, MA), Materials Research Society, 2013.
- MRS 2012 Aravind Krishnamoorthy**, William F. Herbert, and Bilge Yildiz, "Corrosion Reactions on the Pyrite (100) Surface and the Role of Intrinsic Surface Defects", in *MRS Fall Meeting*, (Boston, MA), Materials Research Society, 2012.
- ECS 2012 Aravind Krishnamoorthy**, William F. Herbert, and Bilge Yildiz, "Intrinsic vacancies and corrosion reactivity of the $\text{FeS}_2(100)$ surface", in *ECS PRiME*, (Honolulu, HI), The Electrochemical Society, 2012.