Arjun Kulathuvayal

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Education

Ph.D. Mechanical Engineering *Sept 2021 – Jun 2026*

- Thesis: Optimization of Energy Storage Materials through Ab-initio Calculations and Deep Learning Techniques in Material Science.
- CGPA : **3.92**

College of Aerospace & Mechanical Engineering, The University of Oklahoma, Norman, OK ou.edu/coe/ame
College of Mechanical & Aerospace Engineering, Utah State University, Logan, UT usu.edu/mae

M.S. Physics *July 2017 – May 2019*

- Thesis: Synthesis and Characterization of Strontium Doped Copper Ferrite Nanoparticles.
- **Specialization:** Computational & Condensed Matter Physics

B.S. Physics *July 2014 – May 2017*

- **Minor in:** Mathematics and Chemistry.

Department of Physics, Pondicherry University, Puducherry 605014 India. pondiuni.edu.in/physics

Research Background

Research Intern *Idaho Falls, ID*
Scientific Computing & AI *May – Sept 2025*
Collaborative Computing Center, Idaho National Laboratory (INL)

- Equipped hp adaptivity algorithm in Finite Element framework C++ library, LibMesh.
- Optimized parallel threading capabilities to the algorithm for high performance computing.
- Equipped MOOSE – a nuclear finite element modeling framework (C/C++) with hp adaptivity.

Graduate Research Assistant *Logan, UT*
CMEE Lab, University of Oklahoma/Utah State University *Sept 2021 – May 2025*

- **Graph Variational autoencoders (VAEs)** based Li-ion diffusion mechanism tracking in **Solid Electrolyte Interphase formed on Lithium anode**.
- Training data generation of Li-ion migration profile using **Nudged Elastic Band** methods implemented with Density Functional Theory simulations (DFT).
- **Graph Neural Network** applications in classification/generation of materials.
- Optimization of **2D - MXene** as an auxiliary layer for electrodes to enhance energy storage capabilities using **generative diffusion models**.

Research Intern *Idaho Falls, ID*
Advanced Characterization and Post Irradiation Examination Division *May 2023 – Aug 2023*
Material Fuel Complex, Idaho National Laboratory (INL)

- DFT study on Helium evolution in the lattice of β-$\mathbf{Ga_2O_3}$ under **irradiation** .
- **DFT-Phonon** based simulation study of lattice thermal conductivity change in β-Ga_2O_3 in the presence of Helium in lattice.

Research Intern *Trivandrum, KL, India*
EMERALD Lab, Indian Institute of Space Science and Technology (IIST) *June – July, 2017*

- Fabrication of Metal-Insulator-Metal structure of Zinc oxide 2D-layers using silver as metal electrodes to

develop ReRAM devices using **Spin Vacuum Coating**.

- Weibull distribution analysis to test for the presence **Physically Unclonable Functions**.

M.S. Research & Thesis *Pondicherry, PY, India*
Magnetism and Magnetic Materials Lab, Pondicherry University *July 2018 – May, 2019*

- Thesis: "Synthesis and Characterization of Strontium Doped Copper Ferrite nanoparticles".
- Material characterization using **X-Ray diffraction, Raman, Impedance and I-R Spectroscopy**, and surface characterization using SEM **AFM**.
- DFT study to capture electronic states of strontium doped systems.

Achievements

- **'Outstanding Ph.D. Researcher of the Year'** for the department of Mechanical and Aerospace Engineering, Utah State University. *2024*

Journal Publications

Google scholar: Citations 53 | h-index 2 | i-10 index 1

10. Deep learning assisted modeling of Li-ion transport in SEI: A Graph neural network based study — Jan 2026

    Arjun Kulathuvayal[a], Yanqing Su [b†]

    to be updated

9. Modulation of thermal conductivity of iron-doped β-Ga_2O_3 by helium-ion irradiation. *Journal of Alloys and Compounds (Impact Factor **6.3**)* — Aug 2025

    Arjun Kulathuvayal[a], Ching-heng Shiau, Zilong Hua, Yanqing Su, Di Chen, Ge Yang and Cheng Sun[†]

    https://doi.org/10.1016/j.jallcom.2025.182949

8. Atomic-scale exploration on the local slip resistance of dislocations in body-centred cubic multi-principal element alloys — Jan 2026

    Wu-Rong Jian[a], Henfeng Zhai[a], **Arjun Kulathuvayal**[b], Anshu Raj[b], Yanqing Su[b], Shuozhi Xu[†], Irene J Beyerlein

    https://doi.org/10.1016/j.ijplas.2026.104635

7. Machine learning reveals microbial interactions driving plastic degradation across plastisphere environments — Dec 2025

    Akib Al Mahir1[a], Yunjian Lei[a], **Arjun S Kulathuvayal**[b], Qijun Zhang[b], Luguang Wang[b], Yanqing Su[c], Liyuan Hou[†]

    https://doi.org/10.1016/j.ijplas.2026.104635

6. Interface Catalysts of in-situ Growth TiO2/MXene for Near 100% Faraday Efficiency CO_2 Reduction.*MDPI Molecules (Impact Factor **4.6**)* — Oct 2025

    Shaun Debow, Zichen Shen, **Arjun Kulathuvayal**, Fuzhan Song, Tong Zhang, Haley Fisher, Jesse Brown, Yuqin Qian, Zhi-Chao Huang-Fu, Hui Wang, Zachary Zander, Mark S. Mirotznik, Robert L. Opila, Yanqing Su, and Yi Rao, Yanqing Su[†]

    https://doi.org/10.1016/j.jallcom.2025.182949

5. Grain Size- and Temperature-Dependent Phonon-Mediated Heat Transport in the Solid Electrolyte Interphase: A First-Principles Study *MDPI Modeling (Impact Factor **4.6**)* — Aug 2025

    Arjun Kulathuvayal[a], Yanqing Su[†]

    https://doi.org/10.3390/modelling1010000

4. Elemental diffusion coefficient prediction in conventional alloys using machine learning. *AIP Chemical Physics Reviews (Impact Factor **6.1**)* — Oct 2024

   Arjun Kulathuvayal[a], Yi Rao[b], Yanqing Su[†]

   https://doi.org/10.1063/5.0222001

3. Biochar Reduces the Nanoplastics Uptake by Lettuce and Alleviate Its Toxicity to Plant *(Under review - Journal of Hazardous Materials)* — Jan 2026

   Anwar A. Aly[a], Junjie Tang[a], Mahmoud Zanaty[a], Chanwei Liu[a], Joan McLean[a], Arturo Keller[b], **Arjun Kulathuvayal**[b], Baoshan Xing[b], Yanqing Su[b], Yiming Su[†].

2. Ionic transport through Solid Electrolyte Interphase of Li-ion Batteries: a Holistic Review Spans on the First-Principle Methodologies. *ACS Applied Energy Materials (Impact Factor **9.5**)* — Feb 2023

   Arjun Kulathuvayal[a], Yanqing Su[†]

   https://doi.org/10.1140/epjb/s10051-022-00431-9

1. Effects of ferromagnetism in ab initio calculations of basic structural parameters of Fe-based random binary alloys. *European Physical Journal B (Impact Factor **1.6**)* — Sept 2021

   Shuozhi Xu[a], Liming Xiong[b], **Arjun Kulathuvayal**[b], Yanqing Su[†]

   https://doi.org/10.1140/epjb/s10051-022-00431-9

Conference Publications

2. Adaptive hp refinement on MOOSE through local smoothness and prior error estimate. — Aug 2025

   Arjun Kulathuvayal[a], Roy Stogner, and Alexander Lindsay[†].

   to be updated

1. Anisotropy in Thermal Conductivity of β-Ga_2O_3 under Irradiation: Ab-initio Investigations. — Aug 2023

   Arjun Kulathuvayal[a], Cheng Sun[†].

   https://www.osti.gov/biblio/1995082

Scholarly Presentations

- Poster presentation at TMS (The Minerals, Metals & Materials Society) 2025 Annual Meeting & Exhibition at Las Vegas, Nevada. — *2025*
- USU College of Engineering Poster Session, Spring 2024 — *2024*
- Poster presentations, Summer 2023 and 2025, Idaho National Lab, Idaho Falls Idaho. — *2023*
- Oral presentation, MAE Fall 2023 Seminar Series — *2023*

Teaching Experience

- Teaching Assistant of the courses – Material Science (MAE 2160) and Fluid Mechanics (MAE 3420). — *2021 - 23*

Professional Skills

Programming: C, C++, FORTRAN, Python, SQL, PHP and Javascript.

Computational:

- Expertization with Unix kernel and other Linux environments.
- Expertization in high-performance computing clusters.
- Deep learning (Graph neural network, Auto encoders, Langevin dynamics, generative diffusion models, transformers ...) (ref. my GitHub)
- PyTorch, PyTorch Geometric DeepInv, Tensorflow ...
- Density Functional Theory (VASP, Quantum Espresso)
- CALPHAD simulations for phase diagrams
- Molecular Dynamics (LAMMPS, CP2K)
- Finite Element Methods (MOOSE, dealii, FEniCS)
- AutoCAD, Adobe illustrator, Blender
- Phonon scattering (PhonoPy, ShengBTE, 4-Phonon scattering)
- Web designer - Front end and back end with PHP (Laravel)
- PostgreSQL, API implementation.

Material synthesis/fabrication and instrumentation:

- Physical Vapor Deposition
- Spin Vacuum Coating
- Sol-Gel method
- XRD, SEM, TEM, AFM
- Impedance, UV and Raman spectroscopy
- Positron emission spectroscopy

Leadership/Outreach

- Mentored undergrad students in CMEE lab of Dr. Su at Utah state univ.

Reference personnel

- Yanqing Su
  Asst. professor, Mechanical Engineering
  University of Oklahoma, Norman OK
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- Alexander Lindsay
  MOOSE framework lead
  Idaho National Lab, Idaho Falls, ID
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- Cheng Sun
  Staff scientist, MFC (U510)
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  Mechanical Engineering
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