

Arjun Kulathuvayal

Ph.D. Candidate, Mechanical Engineering, The University of Oklahoma, Norman, OK 73019

✉ arjun.sk@ou.edu ☎ +1 (435)-512 6620 🌐 arjunskv.com

🔗 scholar.google.com/arjuns 🏠 github.com/skvarjun in linkedin.com/arjuns

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 – Present

- **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 -Ga₂O₃ under **irradiation**.
- **DFT-Phonon** based simulation study of lattice thermal conductivity change in β -Ga₂O₃ 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 73 | h-index 3 | i-10 index 1

10. Deep learning assisted modeling of Li-ion transport in SEI: A Graph neural network based study. *Frontiers in Batteries and Electrochemistry* Jan 2026
Arjun Kulathuvayal^a, Yanqing Su ^{b†}
<https://doi.org/10.3389/fbael.2026.1849012>
9. Modulation of thermal conductivity of iron-doped β -Ga₂O₃ 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. *international journal of plasticity Impact Factor 12.8* 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 Mahir^{1a}, 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 CO₂ 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 -Ga₂O₃ 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
yanqing.su@ou.edu
+1 (404) 735-1592
- Alexander Lindsay
Computational scientist
MOOSE framework lead
Idaho National Lab, Idaho Falls, ID
Alexander.Lindsay@inl.gov
+1 (425) 772-9375
- Cheng Sun
Staff scientist, MFC (U510)
Idaho National Lab, Idaho Falls, ID
Associate Professor
Mechanical Engineering
University of Clemson csun2@clemson.edu
+1 (979) 422-0167