Akhil Reddy Peeketi, Ph.D.

peeketiakhilreddy@gmail.com | arpeeketi@lanl.gov

Los Alamos, NM | LinkedIn | ORCID: 0000-0002-9955-7129 | Google Scholar

Research Summary

Computational electrochemistry researcher using **DFT**, **ESM-RISM**, and **ML interatomic potentials** for catalyst mechanisms. At Los Alamos, β-NiOOH OER shown to proceed through pseudocapacitive hydroxyl charge storage, overturning the assumed oxyl pathway, with first-principles XAS matched to operando synchrotron data (*Nature Catalysis*, under review); extended to CoOOH and Cu CO_2 reduction. Built **HIPPIE-NN**, a charge-aware ML potential with Soft-FQEq solver for electrode-electrolyte interfaces. Prior to LANL, built multiscale and multiphysics simulation platforms (FEM, MD, DEM), bringing an infrastructure-builder approach to electrochemistry.

Education

Ph.D., Mechanical Engineering (Best Ph.D. Thesis Award) — July 2019 – May 2024
Indian Institute of Technology Madras, Chennai, India — GPA: 9.33/10
Dissertation: Modeling of Photo/Thermo-Mechanical Actuation in Liquid Crystal Polymers
Advisors: Prof. Ratna K. Annabattula, Prof. Narasimhan Swaminathan

B.Tech & M.Tech (Dual Degree), Mechanical Engineering — July 2014 – May 2019
Indian Institute of Technology Madras, Chennai, India — GPA: 9.39/10

Technical Expertise

First-Principles Catalysis & Surface Phase Diagrams
– DFT methods: **VASP**, **Quantum ESPRESSO**, DFT+U, r^{2}SCAN, NEB transition states
– Phase diagrams: vacuum (CHE) → **ESM-RISM** (implicit solvent) → MLIP-MD (explicit solvent)
– Ab initio thermodynamics, Pourbaix stability, coverage-dependent surface energetics

Operando Validation & Microkinetic Modeling
– **XSpectra** XANES, first-principles spectral simulation, operando synchrotron validation
– Microkinetic modeling (Brønsted–Frumkin coverage-dependent), Tafel slope fitting
– PCET free energy, pseudocapacitive charge storage, dynamic surface evolution

Electronic Structure Analysis
– **COHP/LOBSTER** orbital decomposition, Bader/DDEC6 charge partitioning, DOS/pDOS
– Spin-orbit coupling, charge-disproportionation, structure-property correlation

Machine Learning Potentials & Active Learning
– **HIPPYNN** backbone, **Soft-FQEq** charge-constrained solver, charge-aware MLIP
– Active learning (SOAP-FPS, ensemble UQ), automated DFT-to-ML workflows

Programming, Atomistic Simulation & HPC
– **Python** (ASE, pymatgen), **PyTorch**, FORTRAN, MATLAB, **LAMMPS** all-atom MD
– Custom Parsl execution providers, QE Fortran patches, A100 GPUs (LANL Chicoma)

Research Experience

Postdoctoral Research Associate — May 2024 – Present
Los Alamos National Laboratory, Theoretical Division (T-1)
Mentor: Dr. Travis E. Jones

Electrocatalysis Mechanism & Operando XAS

· Demonstrated pseudocapacitive hydroxyl-mediated OER on β-NiOOH via DFT+U + ESM-RISM; Brønsted–Frumkin kinetics fit operando Tafel slopes (*Nature Catalysis*, under review).

- Simulated O K-edge X-ray absorption spectra for β-NiOOH from first-principles surface terminations (XSpectra); assigned operando BESSY II features to specific coverage states.
- Extended ESM-RISM framework to CoOOH (neutral-pH OER): voltage-dependent surface phase diagrams + potential-dependent O K-edge XAS predictions (528/529 eV) matching operando experiment, with Frumkin-like surface thermodynamics (manuscript in preparation).
- Resolved Cu nanoparticle lattice expansion under CO_2 reduction via ESM-RISM strained-slab surface stress; adsorbate stress dominates over charge contribution (manuscript in preparation).

Electronic Structure & Catalyst Design

- Resolved Pt_3O_4 metallicity via 12-level DFT benchmark + COHP analysis; Pt-O covalency overturns the charge-disproportionation interpretation (*Electron. Struct.* 2026, first author).
- Screened 28 dopants across α/β-PtO_2 ($\sim$168 DFT systems) via automated PBE$\rightarrow$r^{2}SCAN + Pourbaix stability, identifying conducting electrolyzer-support oxides (manuscript in preparation).

ML Potentials & Automated Catalysis Workflows

- Built HIPPIE-NN charge-aware ML interatomic potential: HIPPYNN backbone + augmented-Lagrangian Uzawa solver with per-fragment charge constraints via graph-Laplacian fragment ID; electric double layer emerges from charge-only training (manuscript in preparation).
- Built Python pipeline for catalyst-surface electrochemistry: slab + PZC screening + ESM-RISM constant-charge sweeps; powered all LANL OER and CO_2-reduction DFT campaigns.

Graduate Research Assistant (Ph.D.) July 2019 – May 2024
Indian Institute of Technology Madras
Advisors: Prof. R. K. Annabattula, Prof. N. Swaminathan

Computational Platform & Mentorship

- Built a custom FORTRAN multiphysics FEM platform (UTEMP/UFIELD in Abaqus): solver-within-solver coupling Bubnov–Galerkin thermal FEM with photo-isomerization kinetics through 21 layers; adopted across 4 groups in 3 countries, powered 13 publications.
- Mentored 6 M.S./Ph.D. students at IIT Madras with two co-authored publications (*Soft Matter* 2021, 2025); platform documentation enabled independent adoption by external research groups.

Atomistic Simulation & Theoretical Mechanics

- Developed an all-atom MD framework (LAMMPS, PCFF class2) with a novel probabilistic dihedral switching protocol; in 7,278-atom systems, dynamic cycling drives 15.7% density reduction, disproving the static-geometry hypothesis (*J. Chem. Phys.* 2024).
- Derived closed-form curvature for partially covered bilayer actuators (generalizing Timoshenko 1925); three regimes from one dimensionless parameter m^2n (*Mech. Mater.* 2023).

Inverse Methods & Optimization

- Developed a genetic-algorithm toolkit for inverse two-term kinetic identification from UV-Vis data; built database across 5 polymer compositions (*Polymer* 2025, co-first author).

Graduate Research Assistant (Pre-Ph.D.) June 2017 – February 2020
Indian Institute of Technology Madras
Advisor: Prof. R. K. Annabattula

- Performed the first spatially resolved thermal simulation of a fusion breeder unit ($\sim$12 million particles) using a custom MATLAB FEM solver with ANN surrogates at each Gauss point; revealed 34% spatial variation in effective thermal conductivity for ITER/DEMO blanket design.
- Co-developed shallow ANN (3 layers, R^2=0.99) for granular-bed thermal conductivity (Smoluchowski S-curve captured implicitly); reduced DEM hours to seconds (co-first author).

Research Intern (DAAD-WISE Fellow) May 2017 – July 2017
Karlsruhe Institute of Technology, Germany
Supervisor: Prof. M. Kamlah

Granular Thermal Transport for Fusion Blankets

- Developed a thermal-resistor-network model + MATLAB platform mapping DEM configurations to conductance matrices via Batchelor-O'Brien contact + Smoluchowski rarefied-gas conduction; outperformed four literature models for ceramic breeder pebble beds.
- Derived six analytical correlations for granular-bed thermal conductivity, validated across 8+ ceramics at 25–800°C — widest coverage of any granular-bed ETC model.

Voxel-Based Design Optimization & Automation Dec. 2016 – Jan. 2017
Design Engineering Intern, Caterpillar Inc., India

- Developed a voxel-based MATLAB GUI for fuel tank pickup-point optimization on mining trucks.
- Reduced engineering evaluation from 2 days to 5 minutes via automated voxelization pipeline.

Fellowships & Honors

- **Best Ph.D. Thesis Award** (Prof. PK Raju & Laxmi Endowed Prize), IIT Madras (2024). Selected as the top doctoral research in Mechanical Engineering from 50+ candidates.
- **Prime Minister's Research Fellowship (PMRF)**, Govt. of India (2019–2024). India's most competitive doctoral fellowship (<5% selection rate). Fully funded 5-year doctoral research.
- **Best Oral Presentation**, 8th Asian Conf. on Mechanics of Functional Materials and Structures (ACMFMS-2022), IIT Guwahati. Computational modeling of light-responsive LCN actuators.
- **International Immersion Travel Grant**, IIT Madras (2019). Funded 3-month research visit to Eindhoven University of Technology for collaborative LCN actuator modeling.
- **DAAD-WISE Fellowship**, Govt. of Germany (2017). Research internship at Karlsruhe Institute of Technology for DEM modeling of fusion breeder materials (<10% applicant selection rate).

Publications

22 peer-reviewed articles | 400+ citations | h-index: 12 [Google Scholar]
† - equal contribution as first author.

Published

22. **A. R. Peeketi**, L. Rekhi, A. R. Muñoz, *et al.* "The origin of metallic conductivity in Pt_3O_4: A first principles study." *Electronic Structure* **8**, 015002 (2026).
21. N. C. S. Neeraj, D. Jayoti, **A. R. Peeketi**, R. K. Annabattula. "Multi-wavelength actuation of dual-dye-doped liquid crystal network thin films." *Soft Matter* **21**, 7650–7661 (2025).
20. D. Jayoti†, **A. R. Peeketi**†, R. K. Annabattula. "Isomerization kinetics of azobenzene crosslinked to a liquid crystal polymer network." *Polymer* **339**, 129057 (2025).
19. L. Yue, E. P. J. Ambergen, S. J. D. Lugger, **A. R. Peeketi**, *et al.* "Vacuum thermoforming of optically switchable liquid crystalline elastomer spherical actuators." *Advanced Materials* **36**, 2402559 (2024).
18. **A. R. Peeketi**, E. Joseph, N. Swaminathan, R. K. Annabattula. "Photo-activated dynamic isomerization induced large density changes in liquid crystal polymers: A molecular dynamics study." *J. Chem. Phys.* **160**, 104902 (2024).

17. **A. R. Peeketi**, N. Swaminathan, R. K. Annabattula. "Design of partially covered bilayer thin film actuators." *Mech. Mater.* **187**, 104816 (2023).

16. D. Jayoti†, **A. R. Peeketi**†, *et al.* "Geometry controlled oscillations in liquid crystal polymer films triggered by thermal feedback." *ACS Appl. Mater. Interfaces* **15**, 18362–18371 (2023).

15. **A. R. Peeketi**, J. A. H. P. Sol, N. Swaminathan, *et al.* "Calla lily flower inspired morphing of flat films to conical tubes." *J. Polym. Sci.* **61**, 1065–1073 (2023).

14. D. Jayoti, **A. R. Peeketi**, R. K. Annabattula, S. K. Prasad. "Dynamics of the photo-thermo-mechanical actuations in NIR-dye doped liquid crystal polymer networks." *Soft Matter* **18**, 3358–3368 (2022).

13. M. del Pozo, J. A. H. P. Sol, S. van Uden, **A. R. Peeketi**, *et al.* "Patterned actuators via direct ink writing of liquid crystals." *ACS Appl. Mater. Interfaces* **13**, 59381–59391 (2021).

12. A. Ramgopal, **A. R. Peeketi**, R. K. Annabattula. "Numerical analysis and design of a light-driven liquid crystal polymer-based motorless miniature cart." *Soft Matter* **17**, 7714–7728 (2021).

11. **A. R. Peeketi**, N. Swaminathan, R. K. Annabattula. "Modeling the combined photo-chemo/thermo-mechanical actuation in azobenzene-doped liquid crystal thin films." *J. Appl. Phys.* **129**, 145107 (2021).

10. M. Pilz da Cunha, **A. R. Peeketi**, *et al.* "Light-driven continual oscillatory rocking of a polymer film." *ChemistryOpen* **9**, 1149–1152 (2020).

9. K. Mehta†, **A. R. Peeketi**†, L. Liu†, *et al.* "Design and applications of light-responsive liquid crystal polymer thin films." *Appl. Phys. Rev.* **7**, 041306 (2020). (**Review Article**)

8. R. K. Desu†, **A. R. Peeketi**†, R. K. Annabattula. "Influence of bed conditions on the effective thermal conductivity of ceramic breeder pebble beds using thermal DEM (TDEM)." *Fusion Eng. Des.* **159**, 111767 (2020).

7. K. Mehta, **A. R. Peeketi**, *et al.* "Modeling of surface waves in photo-responsive viscoelastic liquid crystal thin films under a moving light source." *Mech. Mater.* **147**, 103388 (2020).

6. **A. R. Peeketi**, M. Moscardini, S. Pupeschi, *et al.* "Analytical estimation of the effective thermal conductivity of a granular bed in a stagnant gas including the Smoluchowski effect." *Granular Matter* **21**, 93 (2019).

5. M. Pilz da Cunha, **A. R. Peeketi**, *et al.* "A self-sustained soft actuator able to rock and roll." *Chem. Commun.* **55**, 11029–11032 (2019).

4. **A. R. Peeketi**, R. K. Desu, P. Kumbhar, R. K. Annabattula. "Thermal analysis of large granular assemblies using a hierarchical approach coupling the macro-scale finite element method and micro-scale discrete element method through artificial neural networks." *Comput. Part. Mech.* **6**, 811–822 (2019).

3. R. K. Desu†, **A. R. Peeketi**†, R. K. Annabattula. "Artificial neural network-based prediction of effective thermal conductivity of a granular bed in a gaseous environment." *Comput. Part. Mech.* **6**, 503–514 (2019).

2. J. A. H. P. Sol, **A. R. Peeketi**, *et al.* "Butterfly proboscis-inspired tight rolling tapered soft actuator." *Chem. Commun.* **55**, 1726–1729 (2019).

1. **A. R. Peeketi**, M. Moscardini, A. Vijayan, *et al.* "Effective thermal conductivity of a compacted pebble bed in a stagnant gaseous environment: An analytical approach together with DEM." *Fusion Eng. Des.* **130**, 80–88 (2018).

Under Review

– A. Ghafari†, **A. R. Peeketi**†, T. Yadav†, *et al.* "Potential-dependent hydroxyl coverage mediates OER over $NiO_x(OH)_y$." *Nature Catalysis*, under review.

Manuscripts in Preparation

– **A. R. Peeketi**, B. P. Uberuaga, T. E. Jones. "Fragment-constrained charge equilibration for charge-aware machine learning potentials at electrochemical interfaces." *In preparation* (2026).

– T. Götsch, **A. R. Peeketi**, T. E. Jones, *et al.* "The oxygen chemistry during the alkaline OER on cobalt." *In preparation* (2026).

– A. Bergmann, A. Herzog, **A. R. Peeketi**, *et al.* "Lattice strain during CO_2 electroreduction conditions: an *in situ* time-resolved X-ray diffraction study on oxide-derived Cu electrocatalysts." *In preparation* (2026).

Selected Presentations

- **A. R. Peeketi**, B. P. Uberuaga, T. E. Jones. "Fragment-constrained charge equilibration for charge-aware machine learning potentials at electrochemical interfaces." *Poster (Upcoming)*, MLCM 2026, Santa Fe, NM (May 18–21, 2026).
- **A. R. Peeketi**. "From Electrons to Electrocatalysis: Toward Quantitative Predictions of Oxygen Evolution." *Invited Talk*, Oak Ridge National Laboratory, CSED, Oak Ridge, TN (February 2026).
- **A. R. Peeketi**, N. Swaminathan, R. K. Annabattula. "Atomistic simulation of light-induced density changes in azo-LCPs." *7th International Soft Matter Conference*, Osaka, Japan (2023).
- **A. R. Peeketi**, *et al.* "Computational modelling of light-responsive LCN thin films." *8th Asian Conf. Mechanics of Functional Materials and Structures*, IIT Guwahati (2022). **[Best Oral]**
- **A. R. Peeketi**, N. Swaminathan, R. K. Annabattula. "Computational modeling of stimuli-responsive bilayer actuators." *18th European Mechanics of Materials Conf.*, Oxford, UK (2022).

Mentorship & Professional Service

- **Graduate Student Mentorship:** Mentored 6 M.S./Ph.D. students on multiscale simulation methodology; 2 co-authored publications; frameworks adopted by 3 international research groups.
- **Teaching:** NPTEL Teaching Assistant for "Machinery Fault Diagnosis and Monitoring" and "Basics of Material Engineering" online courses (2022–23); 500+ enrolled students across two semesters.
- **Peer Review:** Reviewer for journals including *Journal of Catalysis*, *Journal of the American Chemical Society*, and *Journal of Applied Physics* (2025–2026).

International Collaborations

- **Fritz Haber Institute & MPI-CEC, Germany** (2024–Present): DFT phase diagram validation against operando XAS with Dr. D. Teschner.
- **Eindhoven University of Technology** (2018–2024): Six-year collaboration on LCE multiphysics; 8 co-authored publications with Prof. A. Schenning, Prof. M. Debije.
- **Karlsruhe Institute of Technology & University of Sydney** (2017–2020): DEM thermal modeling for fusion blankets with Prof. M. Kamlah and Prof. Y. Gan; 3 publications.
- **University of Groningen** (2019–2020): Photo-responsive polymer modeling with Prof. P. Onck.