Manish K. Kothakonda

190 Mountain Ave,
Malden, MA
m.kothakonda@northeastern.edu
+1-504-535-8853

Education

Tulane University, New Orleans, Louisiana, USA — Jan'16 - Aug'22
Doctor of Philosophy, Physics

University of Hyderabad, Hyderabad, Telangana, INDIA — Aug'09 - May'14
Integrated Masters of Science, Physics

Area of Expertise

Density functional theory(DFT), Computational Catalysis, Reaction path and barrier calculation, Electronic structure calculations, Machine Learning, Dimensionality reduction, clustering, Deep Learning, Data visualization, PCA, t-SNE, Unix/Linux , HPC Cluster

Computational Skills

Languages: Python, FORTRAN, Bash, LATEX
python lib: sklearn, matminer, Pymatgen, ASE, Phonopy, Pandas, NumPy,Matplotlib, Jupyter-Notebook, Plotly
Modeling & Simulation Software: VASP, GW, and LAMMPS

Work Experience

Post-Doctoral Researcher Associate — Sept'23 - Present
(Northeastern Univertsity) Advisor: Dr. Qing Zhao

Design and Optimization of Single Atom Alloy Catalysts for Methane Activation

- Designed and evaluated 30 transition metal-based Single Atom Alloy (SAA) configurations for catalytic studies using computational tools.
- Applied Density Functional Theory (DFT) to optimize catalytic processes, focusing on methane activation, coke mitigation, and selectivity towards C2 products.
- Assessed structural stability and investigated kinetics and thermodynamics of SAA catalysts, identifying promising candidates with high activity and selectivity.
- Mentored undergraduate and graduate students in ab-initio DFT calculations, enhancing their skills in computational catalysis.

Post-Doctoral Researcher — Sept'22 - Aug' 23
(Colorado School of Mines & NREL) Advisor: Dr. Prashun Gorai

Semiconductors Project: Designing New semiconducting zintl Phases with Motif based GNN and Ab Initio Methods

- Compiled a comprehensive database of naturally occurring Zintl compound prototypes, expanding it to ~90,000 compounds by decorating prototypes with all possible elements.
- Optimized a Graph Neural Network (GNN) model by tuning hyperparameters based on DFT volume-only relaxed energies, achieving a 99% reduction in prediction time for structure stability.
- Predicted and validated 1,810 stable structures using full relaxation DFT, identifying 1,000 potentially thermodynamically stable Zintl structures for experimental synthesis by collaborators.
- Leveraged data-driven computational chemistry to explore the vast chemical space of Zintl phases, discovering 1,810 new stable phases through efficient scanning and accurate predictions.

Battery Project: DFT to predict defect and doping properties of solid electrolytes for solid-state batteries.

- Conducted computational modeling of disordered phases of Li3MCl6 solid electrolyte materials using DFT.
- Calculated formation energies of defects and aliovalent dopants to identify dominant defects, dopants, and optimal synthesis conditions.
- Analyzed the relationship between Li-vacancy concentration, aliovalent dopant concentration, and dominant native defect concentration to determine the impact on the ionic conductivity of Li-Metal Halide solid electrolyte.
- Generated a grand potential phase diagram to gain insight into the electrochemical stability window of Li-Metal Halide solid electrolyte when used with Li-Metal as an anode.

Research Experience

Graduate Research Assistant
(Tulane University) Advisor: Dr. Jianwei Sun
Oct'17 - Aug'22

Method Development: Design, Optimize and Test novel density functional Opt(MS+rVV10) for adsorption energy benchmarks

- Designed a new density functional implemented in VASP to increase the accuracy of adsorption energies of heterogeneous catalysis by novel mathematical formulation specifically optimized to understand the bonding properties and varying bond density regions of heterogeneous adsorption
- This optimized functional was tested against various organic molecules adsorbed on transition metal surfaces and has improved overall error for the adsorption energies compared with the most accurate functional until now.
- Manuscript under review in Nature Catalysis, Link to APS March Meeting: Link

High-throughput testing: Testing r2SCAN density functional for the thermodynamical stability of solids with and without the van der Waals correction

- Tested, and analyzed the performance of r2SCAN density functional for a set of 2500 solid state materials consisting of 84 elements of the periodic table, which include various binaries, ternaries, and quaternary
- Calculated thermodynamic properties such as formation and decomposition energies of a set of 2500 solids using r2SCAN, SCAN, and rVV10 counterparts and compared with Factsage experimental data
- Compared the performance of density functionals for properties such as bandgaps, magnetism, and volumes
- Automated the testing and visualization process using state-of-the-art python libraries such as pandas, numpy, pymatgen, ase, and matplotlib
- Published article: doi:10.1021/acsmaterialsau.2c00059 ACS Materials Au

2D Materials Discovery: High-throughput screening assisted discovery of stable Anti-ferromagnetic semiconductor: CdFeP2Se6

- Accurately predicted symmetry of the structure, magnetic structure, and electronic structure
- Experimentally measured and Theoretically confirmed novel anti-ferromagnetic semiconductor properties
- Published article: doi:/10.1002/adfm.202210965 Advanced Functional Materials (2023): 2210965

TMCC: Transition Metal Carbo-Chalcogenide "TMCC" A New Family of 2D Materials

- Modeled a new family of 2D materials which is a blend of MXenes and TMDs
- Accurately predicted thermodynamic stability and electronic properties for understanding the energy storage properties
- Published article: doi: 10.1002/adma.202200574 Advanced Materials 34.26 (2022): 2200574

Teaching Experience

Graduate Teaching Assistant
(Tulane University) Supervisor: Dr. Timothy M. Schuler
Aug'17 - May'20

- Taught the Great Ideas in Science and Technology PHYS-1010, Introductory Physics I PHYS-1211, General Physics lab I PHYS-1310 and II PHYS-1320 during Fall and Spring semesters - Grading lab reports, and assignments and recording the student´s performance by maintaining a database
- Training of students in lab experiments, quality procedures, data analysis, and interpretation
- Actively participated in preparing innovative lesson plans
- Graded undergraduate course Mechanics of Materials ENGP 2430 and graduate level course Electronic Properties of Materials PHYS-3700.
- Delivered invited guest lectures according to the course needs during the travel appointments of professors for Mechanics of Materials and Electronic Properties of Materials.

Professional Activities

Reviewer: RSC Energy Advances, Nature Computational Materials, Journal of Chemical Theory and Computation, Physical Review B, Multidisciplinary Digital Publishing Institute(Molecules, Crystals, and Materials)

Awards& Achievements

- Cleared FE Chemical Engineering certification from Louisiana NCEES board (Link)
- Received Tulane GSSA travel awards totaling $5,000 to present research at the American Physical Society (APS) March Meetings in 2019, 2021, and 2022.
- Received a $6,000 INSPIRE Scholarship from the Department of Science and Technology, Government of India, for pursuing an Integrated Masters in Physics from 2009 to 2014.
- Granted a $15,000 Summer Internship Program for Indian Students (SIPIS) at the National University of Singapore in 2014.
- Awarded a $5,000 Indian Science Academies Summer Research Fellowship at IIT Bombay in 2012.

Publications

1. **Kothakonda, M.**, Sarah LaCroix, Ji Su, Qing Zhao Exploring Single Atom Alloy Catalysts for Enhanced Methane Activation to C2+ Products: Insights from Computational Modeling under preparation
2. **Kothakonda, M.**, Ji Yang, Yi Chena,1, Malavika Bagepallia, Jiayun Liangd, Jiawei Wane, Xiao Zhaoe, Xianhu Sune, Daniel Hawthornea, Zengqing Zhuof, Grace Laua, Jinghua Guof, Haimei Zhenge, Miquel Salmerone, Zakaria Al Balushid, Zhao, Q., Ravi Prashera*, Ji Sua*, Sumanjeet Kaura* "Cerium Hydrides Promoted CO2 Methanation over Ni-CeO2/Al2O3 Catalysts" under review
3. Gallagher, C., **Kothakonda, M.**, Zhao, Q. "Graphene-Based Single-Atom Catalysts for Electrochemical CO2 Reduction: Analyzing Mechanistic Pathways and Conventional Descriptors for Predicting Activity" under review ACS Catalysis
4. **Kothakonda, M.**, C-W. Lee, J. Law, P. Gorai "Charting the Large Chemical Space of Zintl Phases using Graph Neural Networks" MRS talk: Link, Manuscript under preparation
5. **Kothakonda, M.**, S. R. Combs, A. E. Maughan, P. Gorai "Prediction and Insights into Aliovalent Doping of Solid Electrolytes: Case of Li_3MCl_6 (M = Sc, Y)}" under review
6. **Kothakonda, M.**, A. Kaplan, E. Isaacs, C. J. Bartel, J. Furness, J. Ning, J. Perdew, C. Wolverton, J.Sun "Testing the r2SCAN density functional for the thermodynamical stability of solids with and without the van der Waals correction" ACS Materials Au : https://doi.org/10.1021/acsmaterialsau.2c00059
7. **Kothakonda, M.**, Y. Zhu, Y. Guan, J.Ning, R. Zhang, W. Xie, Z. Mao, Sun J. 2022 "High-throughput screening assisted discovery of stable Anti-ferromagnetic semiconductor: CdFeP2Se6" Advanced Functional Materials https://doi.org/10.1002/adfm.202210965
8. **Kothakonda, M.**, Zhang R., Ning J. Furness J. W., Sun J. 2022 "An efficient density functional for accurate molecular chemisorption and physisorption on transition metal surfaces" under review nature catalysis
9. A. Majed, **Kothakonda, M.**, F. Wang, E.N. Tseng, K. Prenger, P. O. A. Persson, J. Wei, J. Sun, M. Naguib 2022 " Transition Metal Carbo-Chalcogenide "TMCC" a New Family of Two-dimensional Materials" Advanced Materials https://doi.org/10.1002/adma.202200574
10. Ning, J., **Kothakonda, M.**, Furness, J.W., Kaplan, A.D., Ehlert, S., Brandenburg, J.G., Perdew, J.P., and Sun, J. "Workhorse minimally empirical dispersion-corrected density functional tested for dimers and layered materials: r2SCAN+rVV10" Physical Review B https://journals.aps.org/prb/abstract/10.1103/PhysRevB.106.075422
11. Y. D. Guan, S. H. Lee, X. Gui, **Kothakonda, M.**, Ning, J., Sun, J. Zhiqiang, M. 2021."Ferromagnetic MnBi 4Te7 obtained with low-concentration Sb doping: A promising platform for exploring topological quantum states" Physical Review Materials https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.6.054203
12. Kun L., Tabassum A., **Kothakonda M.**, Zhang X., Zhang R., Kenney B.,Koplitz B.T., Sun J., Naguib M. 2021. "Two-Dimensional Titanium Carbonitride MXene as a Highly Efficient Electrocatalyst for Hydrogen Evolution Reaction" Materials Reports: Energy https://doi.org/10.1016/j.matre.2021.100075
13. Puli, V.S., Ejaz, M., Elupula, R., **Kothakonda, M.**, Adireddy, S., Katiyar, R.S., Grayson, S.M. and Chrisey, D.B., 2016."Core-shell like structured barium zirconium titanate-barium calcium titanate–poly (methyl methacrylate) nanocomposites for dielectric energy storage capacitors" Polymer https://doi.org/10.1016/j.polymer.2016.10.020
14. Puli, V.S., Pradhan, D.K., Adireddy, S., **Kothakonda, M.**, Katiyar, R.S. and Chrisey, D.B., 2016. "Effect of lead borosilicate glass addition on the crystallization, ferroelectric and dielectric energy storage properties of Ba0. 9995La0. 0005TiO3 ceramics" Journal of Alloys and Compounds https://doi.org/10.1016/j.jallcom.2016.07.025
15. Puli, V.S., Adireddy, S., **Kothakonda, M.**, Elupula, R. and Chrisey, D.B., 2017. "Low temperature sintered giant dielectric permittivity CaCu3Ti4O 1 2 sol-gel synthesized nanoparticle capacitors" Journal of Advanced Dielectrics https://doi.org/10.1142/S2010135X17500175
16. **Kothakonda, M.**, Bourgeois, B., Riggs, B.C., Puli, V.S., Elupula, R., Ejaz, M., Adireddy, S., Grayson, S.M. and Chrisey, D.B., 2018. "Core-Shell Nanoparticles for Energy Storage Applications. In Pulsed Laser Ablation" CRC Press