Manish K. Kothakonda

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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

Physics informed Machine Learning, Density functional theory(DFT), Quantum chemistry, Computational Material Sciences, Reaction path prediction, Crystal Structure Prediction, Electronic structure calculations, Dimensionality reduction, clustering, Deep Learning, Data visualization, PCA, t-SNE, Data mining, ab-initio studies, Unix/Linux , HPC Cluster

Computational Skills

Languages: Python, Julia, C, MATLAB, FORTRAN, Bash, LATEX
python lib: sklearn, matminer, Pymatgen, ASE, Phonopy, Pandas, NumPy,Matplotlib, Jupyter-Notebook, Plotly
Modeling & Simulation Software: VASP, PC-SAFT, UNIFAC, GW, and LAMMPS
Database prog: SQL, MySQL

Work Experience

Post-Doctoral Researcher Associate (Northeastern Univertsity) — Sept'23 - Present

Computational Catalysis Researcher with Expertise in Physics-Informed Machine Learning

- Pioneered physics-informed machine learning in catalysis research, enhancing predictive simulations and enabling rapid screening of over 550 Single Atom Alloy (SAA) configurations.
- Applied density functional theory calculations and computational tools to optimize catalytic processes for enhanced selectivity towards C2 products.
- Expertly mitigated coke formation and improved selectivity in catalytic reactions through rigorous analysis and computational tools.
- Developed novel reaction pathways for new SAAs with improved kinetics, accelerating material discovery through predictive simulations and machine learning insights.

Work Experience

Post-Doctoral Researcher (NREL & Colorado School of Mines) — Sept'22 - Aug' 23

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.
- Expanded the database by decorating prototypes with all possible elements, resulting in 95,000 compounds.
- Optimized the Graph Neural Network model by tuning hyperparameters based on DFT volume-only relaxed energies of a 5% decoration set.
- The GNN based machine learning algorithm that achieved a remarkable 99% reduction in the time required to predict the stability of structure prototypes.
- Predicted and validated 1,200 stable structures out of 90,000 using full relaxation DFT, and identified 1,000 potentially thermodynamically stable decorated zintl structures using UNIFAC for experimental synthesis by collaborators.

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 (VASP).
- 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)

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.

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

- Thermodynamically PC-SAFT screened a new family of 2D materials by calculating reaction-free energies
- 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)

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)
- **Member:** Americal Physical Society(APS) (2018 - Present), American Chemical Society(ACS) (2020 - Present), Materials Research Scociety(MRS) (2020 - Present), American Institure of Chemical Engineers(AICHe) (2024 - Present)

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.,** C-W. Lee, J. Law, P. Gorai "Discovering Large Families of Zintl Phases using Graph Neural Networks" under review JACS: **https://chemrxiv.org/engage/chemrxiv/article-details/60c7579dbb8c1a48b63dc892**
2. **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
3. **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**
4. **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**
5. **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**
6. 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**
7. 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**
8. 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**
9. 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**
10. 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**
11. 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**
12. 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**
13. **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**