

Manish K. Kothakonda

Curriculum Vitae

Department of Chemical Engineering
Northeastern University
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Education

- 2016–2022 **Ph.D., Physics(Materials Track), Tulane University**, New Orleans, Louisiana, USA.
Advisor Jianwei Sun
Dissertation Electronic, Magnetic, Structural and Energetic Properties of 2D Materials, Solids and Surface/Interfaces with Applications for Catalysis and Optoelectronics
- 2009–2014 **Integrated(BS+MS), Physics, University of Hyderabad**, Hyderabad, Telangana, INDIA.
Thesis Nanoparticles/nanostructures assisted surface enhanced Raman spectroscopy: Detection of oxidative stress in THP1 monocytes

Expertise & Skills

- Github Link <https://github.com/manishkothakonda>
- Area of Expertise Computational Catalyst design, ab-initio Density functional theory, Molecular dynamics, CO₂ reduction reaction, CH₄ dehydrogenation to C₂+ products, Reaction barrier & path prediction, and Structure stability prediction(convex hull)
- Coding Python, FORTRAN90, C/C++, CMake, Bash, MPI, OpenMPI, and L^AT_EX
- Python libraries sklearn, matminer, Pymatgen, ASE, Phonopy, Pandas, NumPy, Matplotlib, Jupyter-Notebook, and Plotly
- Ab-initio & MD Tools VASP, cp2k, GPAW, Molpro, TeraChem, Quantum Espresso, and LAMMPS
- Datascience Graph Neural Network, Dimensionality reduction ,PCA, t-SNE, and DB-SCAN

Research Experience

- Sept 2023 – **Post-Doctoral Research Associate**, CHEMICAL ENGINEERING, NORTHEASTERN UNIVERSITY, Boston, MA.
Current
Advisor Qing Zhao
- * Designed and evaluated 30 transition metal-based Single Atom Alloy (SAA) configurations for catalytic studies using advanced computational tools. Through Density Functional Theory (DFT) calculations, catalytic processes were optimized with a focus on methane activation, coke mitigation, and selectivity towards C₂ products. The work involved a comprehensive assessment of structural stability, kinetics, and thermodynamics of SAA catalysts, identifying highly active and selective candidates. Additionally, ab-initio molecular dynamics (AIMD) was employed to explore reaction sites and the solvation effects of water using both implicit and explicit solvation models for the electrochemical conversion of CH₄ to C₂ products, providing deeper insights into electrochemical reaction mechanisms.
 - * I developed machine-learned interatomic potentials (MLIPs) to replicate ab initio QM/MM calculations for enzyme-catalyzed reactions, using techniques like deep neural networks (DNN) and kernel ridge regression (KRR). This work focused on modeling both local and long-range interactions and was benchmarked across enzymes such as chorismate mutase and HIV-1 protease, improving predictions of reaction energetics and conformational dynamics.

Sept 2022 – **Post-Doctoral Research Associate**, MATERIALS SCIENCE & ENGINEERING, COLORADO
Sept 2023 SCHOOL OF MINES & NATIONAL RENEWABLE ENERGY LAB, Golden, CO.

Advisor Prashun Gorai

Compiled a database of 90,000 Zintl compound prototypes by decorating naturally occurring structures. Trained a Graph Neural Network (GNN) model on DFT-relaxed energies, predicting 1,836 stable structures. Validated 1,636 thermodynamically stable candidates with 90% GNN accuracy, leveraging data-driven dimensionality reduction to discover novel Zintl materials.

2016 – 2022 **Graduate Research Assistant**, PHYSICS AND ENGINEERING PHYSICS, TULANE UNIVERSITY, New Orleans, LA.

Advisor Jianwei Sun

Worked on multiple projects, including developing and optimizing the Opt(MS+rVV10) density functional for adsorption energy benchmarks and testing the r2SCAN functional for thermodynamic stability of solids with and without van der Waals corrections. Conducted high-throughput screening for 2D materials, leading to the discovery of a stable anti-ferromagnetic semiconductor, CdFeP₂Se₆, and explored the new family of 2D materials known as Transition Metal Carbo-Chalcogenides (TMCC).

Teaching

Responsibilities included grading lab reports and assignments, maintaining a performance database, and training students in lab experiments, data analysis, and interpretation. Held office hours, proctored and graded exams, managed undergraduate teaching assistants, and assisted during class.

Fall 2017 **PHYS 1310**, *General Physics lab I*, Teaching Assistant.

Under Prof. Timothy M. Schuler

Spring 2018 **PHYS 1320**, *General Physics lab II*, Teaching Assistant.

& 2019 Under Prof. Timothy M. Schuler

Fall 2019 **PHYS 1211**, *Introductory Physics I*, Teaching Assistant.

Under Prof. Timothy M. Schuler

Spring 2020 **PHYS 1010**, *Great Ideas in Science and Technology*, Teaching Assistant.

Under Prof. Timothy M. Schuler

Fall 2021 **PHYS 3700**, *Electronic Properties of Materials*, Teaching Assistant & Grader.

Under Prof. Zhiqiang Mao

Mentorship

Spring 2024 – **Sarah LaCroix**

Current Undergraduate Northeastern University, Independent Research, Supervised by Qing Zhao, Understanding Ru-based single atom alloys for ammonia decomposition.

Fall 2023 & **Carmen Cheng**

Spring 2024 Undergraduate Northeastern Independent Research, Supervised by Qing Zhao, Benchmarking a Molecular Flake Model on the Road to Programmable Graphene-Based Single-Atom Catalysts.

Summer 2020 **Elena Lompado**

Undergraduate Tulane, Independent Research, Supervised by Jianwei Sun, Predicting Free Energies of Transition Metal-Based XY₂Se₄ Compounds for Semiconductor Applications.

Reviewer

Jan 2023 - RSC Energy Advances, Nature Computational Materials, Journal of Chemical Theory and
Current Computation, Physical Review B, and Multidisciplinary Digital Publishing Institute(Molecules,
Crystals, and Materials)

Publications

Google Scholar <https://scholar.google.com/citations?user=chmsWhIAAAAJ&hl=en>

- 2024 Towards chemical accuracy for chemi- and physisorption with an efficient density functional, **Kothakonda, Manish, Zhang R., Ning J. Furness J. W., Patra Abhirup, Zhao Qing, Sun Jianwei, under review Nature Catalysis.**
[arXiv Link](#)
- 2024 Exploring Single Atom Alloy Catalysts for Enhanced Methane Activation to C2+ Products: Insights from Computational Modeling, **Kothakonda, Manish, Sarah LaCroix, Ji Yang, Ji Su, Qing Zhao, under review JACS.**
[arXiv Link](#)
- 2024 Cerium Hydrides Promoted CO2 Methanation over Ni-CeO2/Al2O3 Catalysts, **Kothakonda, Manish, Ji Yang, Yi Chen, Malavika Bagepalli, Jiayun Liang, Jiawei Wan, Xiao Zhao, Xianhu Sun, Daniel Hawthorn, Zengqing Zhuo, Grace Lau, Jinghua Guo, Haimei Zheng, Miquel Salmeron, Zakaria Al Balushi, Zhao, Qing*, Ravi Prasher*, Ji Su*, Sumanjeet Kaur*, under review Angewandte Chemie.**
[Link](#)
- 2024 Graphene-Based Single-Atom Catalysts for Electrochemical CO2 Reduction: Analyzing Mechanistic Pathways and Conventional Descriptors for Predicting Activity, *Gallagher, C., Kothakonda, Manish, Zhao, Q, under review ACS Catalysis.*
- 2024 Charting the Large Chemical Space of Zintl Phases using Graph Neural Networks, **Kothakonda, Manish, C-W. Lee, J. Law, P. Gorai, under review JACS.**
<https://www.mrs.org/meetings-events/annual-meetings/archive/meeting/presentations/view/2023-mrs-fall-meeting/2023-mrs-fall-meeting-3959202>
- 2023 High-throughput screening assisted discovery of stable Anti-ferromagnetic semiconductor: Cd-FeP2Se6, **Kothakonda, Manish, Y. Zhu, Y. Guan, J. Ning, R. Zhang, W. Xie, Z. Mao, Sun J. , Advanced Functional Materials 33.9 (2023): 2210965.**
<https://doi.org/10.1002/adfm.202210965>
- 2022 Two-Dimensional Titanium Carbonitride MXene as a Highly Efficient Electrocatalyst for Hydrogen Evolution Reaction, *Kun L., Tabassum A., Kothakonda, Manish, Zhang X., Zhang R., Kenney B., Koplitz B. T., Sun J., Naguib M., Materials Reports: Energy 2.1 (2022): 100075.*
<https://doi.org/10.1016/j.matre.2021.100075>
- 2022 Testing the r2SCAN density functional for the thermodynamical stability of solids with and without the van der Waals correction, **Kothakonda, Manish, A. Kaplan, E. Isaacs, C. J. Bartel, J. Furness, J. Ning, J. Perdew, C. Wolverton, J. Sun, ACS Materials Au 3.2 (2022): 102-111.**
<https://doi.org/10.1021/acsmaterialsau.2c00059>
- 2022 Transition Metal Carbo-Chalcogenide "TMCC" a New Family of Two-dimensional Materials, *A. Majed, Kothakonda, Manish, F. Wang, E.N. Tseng, K. Prenger, P. O. A. Persson, J. Wei, J. Sun, M. Naguib, Advanced Materials 34.26 (2022): 2200574.*
<https://doi.org/10.1002/adma.202200574>

- 2022 Workhorse minimally empirical dispersion-corrected density functional tested for dimers and layered materials: r2SCAN+rVV10, *Ning, J., **Kothakonda, Manish**, Furness, J.W., Kaplan, A.D., Ehlert, S., Brandenburg, J.G., Perdew, J.P., and Sun, J.*, **Physical Review B** **106.7** (2022): 075422.
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.106.075422>
- 2022 Ferromagnetic MnBi4Te7 obtained with low-concentration Sb doping: A promising platform for exploring topological quantum states, *Y. D. Guan, S. H. Lee, X. Gui, **Kothakonda, Manish**, Ning, J., Sun, J. Zhiqiang, M.*, **Physical Review Materials** **6.5** (2022): 054203.
<https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.6.054203>
- 2018 Core-Shell Nanoparticles for Energy Storage Applications., **Kothakonda, Manish**, *Bourgeois, B., Riggs, B.C., Puli, V.S., Elupula, R., Ejaz, M., Adireddy, S., Grayson, S.M. and Chrisey, D.B.*
<https://www.taylorfrancis.com/chapters/edit/10.1201/9781315185231-8/core-shell-nanoparticles-energy-storage-applications-manish-kothakonda-briley-bourgeois-bri>
- 2017 Low temperature sintered giant dielectric permittivity CaCu3Ti4O12 sol-gel synthesized nanoparticle capacitors, *Puli, V.S., Adireddy, S., **Kothakonda, Manish**, Elupula, R. and Chrisey, D.B.*
<https://doi.org/10.1142/S2010135X17500175>
- 2016 Core-shell like structured barium zirconium titanate-barium calcium titanate-poly (methyl methacrylate) nanocomposites for dielectric energy storage capacitors, *Puli, V.S., Ejaz, M., Elupula, R., **Kothakonda, Manish**, Adireddy, S., Katiyar, R.S., Grayson, S.M. and Chrisey, D.B.*
<https://doi.org/10.1016/j.polymer.2016.10.020>
- 2016 Effect of lead borosilicate glass addition on the crystallization, ferroelectric and dielectric energy storage properties of Ba0.9995La0.0005TiO3 ceramics, *Puli, V.S., Pradhan, D.K., Adireddy, S., **Kothakonda, Manish**, Katiyar, R.S. and Chrisey, D.B.*
<https://doi.org/10.1016/j.jallcom.2016.07.025>

Presentations & Posters

- March 2019 Benchmark studies for adsorption bond energies to transition metal surfaces, **Manish Kothakonda**, *Jinliang Ning, Yubo Zhang, James Furness, Jianwei Sun*, Oral presentation, Boston, MA.
<https://ui.adsabs.harvard.edu/abs/2019APS..MARL31007K/abstract>
- March 2020 How accurate can a metaGGA+ vdW functional be simultaneously for chemisorption and physisorption of molecular adsorption on transition metal surfaces?, **Manish Kothakonda**, *Jinliang Ning, Yubo Zhang, James Furness, Jianwei Sun*, Oral presentation, Denver, CO.
<https://meetings.aps.org/Meeting/MAR20/Session/F58.8>
- March 2021 An efficient density functional for accurate molecular chemisorption and physisorption on transition metal surfaces, **Manish Kothakonda**, *Jinliang Ning, Yubo Zhang, James Furness, Jianwei Sun*, Oral presentation, Online.
<https://ui.adsabs.harvard.edu/abs/2021APS..MARJ20015K/abstract>
- Oct 2024 Exploring Single Atom Alloy Catalysts for Enhanced Methane Activation to C2+ Products: Insights from Computational Modeling, **Manish Kothakonda**, *Sarah LaCroix, Qing Zhao*, Poster presentation, Online.
<https://aiche.confex.com/aiche/2024/meetingapp.cgi/Paper/690527>

Honors & Awards

- 2024 **Travel fellowship for Workshop & Panel on FAIR Workflows in Materials Science**, *Department of Materials Engineering, Purdue University*.
 Fellowship awarded by the Purdue University for attending workshop
- 2019, 2021, & 2022 **GSSA Travel award to attend APS March meeting**, *Department of Physics and Engineering Physics, Tulane University*.
 Travel award by the Tulane University for attending conference given to 4/20

- 2009-2014 **Innovation in Science Pursuit for Inspired Research (INSPIRE)**, *Department of Science and Technology(DST), Govt. of India.*
Fellowship awarded by the DST government of India for excelling in competitive exams
- 2014 **Summer Internship Program for Indian Students**, *National University of Singapore(NUS), Singapore.*
Scholarship awarded by the National University of Singapore for doing research at NUS
- 2012 **Indian Science Academies Summer Research Fellowship**, *Indian Institute of Technology, Bombay.*
Fellowship awarded to rising sophomores for conducting research over the summer