Kamal Choudhary, Ph.D.

Email: kchoudh2@jhu.edu | **Google Scholar:** scholar.google.com/citations?user=klhV2BIAAAAJ
GitHub: github.com/atomgptlab | **YouTube:** youtube.com/@dr_k_choudhary

SUMMARY OF QUALIFICATIONS

Research

- Computational materials scientist with 14+ years of experience in multiscale modeling, uncertainty quantification, and AI-driven materials discovery.
- Developer and maintainer of the **NIST-JARVIS infrastructure** with **>200,000 users worldwide**.
- Developer and maintainer of AtomGPT.org & **ChatGPT Material Explorer** with ~10000 users.
- **>100 peer-reviewed publications** with ~**10,000 citations** and an **h-index of 47**.
- Open datasets downloaded ~3 million times (Figshare).
- Presented **50+ invited talks** at conferences and symposia.
- Interdisciplinary collaborator with experience in **computational and experimental materials design**.
- Developed **open-access 11+ AI/ML packages**: https://github.com/atomgptlab

  AGAPI, InterMat, SlaKoNet, DefectMat, AtomGPT, DiffractGPT, MicroscopyGPT,ALIGNN, ChemNLP, AtomVision, TB3Py, CHIPSFF, SLMat, BenchQC, JARVIS-Leaderboard, JARVIS-tools.

Teaching & Mentorship

- Assistant Professor, Department of Materials Science and Engineering, Electrical and Computer Engineering
- Adjunct Professor, Engineering for Professionals program, Mechanical Engineering, Johns Hopkins University.
- Designed and taught the Multiscale Modeling and Simulation of Mechanical Systems course.
- Mentored 6 postdoctoral researchers and 9 Ph.D. students.

Service & Leadership

- Associate Editor: npj Computational Materials (Nature Publishing Group).
- Editorial team member: Materials Today Communications, PRX Energy, Scientific Data
- CEO and founder of a small business DeepMaterials LLC
- Organizer of Artificial Intelligence for Materials Science (AIMS), Quantum Matters in Materials Science (QMMS) workshops, and JARVIS-School tutorials.
- Active member of TMS, APS, and MRS societies.

EDUCATION

UNIVERSITY OF FLORIDA
Gainesville, Florida, August 2015
Doctor of Philosophy (Ph.D.) Material Science and Engineering

- Thesis: Computational Design of Surfaces, Nanostructures and Optoelectronic Materials

- Advisor: Dr. Susan B. Sinnott

UNIVERSITY OF FLORIDA
Gainesville, Florida, May 2013
Master of Science (MS) in Material Science and Engineering

GOVERNMENT COLLEGE OF ENGG. AND CERAMIC TECHNOLOGY *Kolkata, India, May 2011*
Bachelor of Technology (B. Tech) in Ceramic Technology
- Thesis: Experimental & Finite Element Simulation Study of Nanoindentation of Hydroxyapatite

WORK EXPERIENCES

JOHNS HOPKINS UNIVERSITY
Baltimore, MD, July. 2025–Aug. present
Assistant Professor
- Developed ChatGPT Material Explorer
- Developed AtomGPT.org
- Developed DiffractGPT, MicroscopyGPT
- Started AtomGPTLab

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
Staff-scientist
Gaithersburg, MD, Dec. 2015 – June 2025
- Atomistic Generative Pretrained Transformer: AtomGPT
- Graph neural network model development for atomistic data: ALIGNN,
- Transformer models for text data: ChemNLP
- Convolution neural network model for image data: AtomVision
- Traditional ML descriptor model: CFID
- Benchmarking AI/ML and other methods: JARVIS-Leaderboard,
- Direct Air/CO_2 Capture using AI model and webapp development
- Core developer of Joint Automated Repository for Various Integrated Simulations (JARVIS) database
- Quantum algorithm application for materials design using AtomQC
- Evaluation of classical-force fields
- Computational screening and optimization of functional materials such as 2D, topological, superconductor, piezoelectric, dielectric, thermoelectrics, high-hardness, solar cell materials
- Electronic structure calculations: density functional theory (DFT)
- Collaborator with various higher education institutions for JARVIS School and taught workshops and sessions related to material science and materials discovery
- Led tutorial in American Physical Society GDS tutorial
- Led tutorial at NSF PARADIM
- Partnered with CHIMAD at Northwestern University on AI-based material design

UNIVERSITY OF FLORIDA
Gainesville, FL, Aug. 2011–Aug. 2015
Research Assistant
- Developed classical force-fields
- Worked on surface chemistry of polymers

- Heterostructure design for metal-ceramic interface
- Optoelectronic properties of lanthanide-substituted systems
- Mentored junior graduate students

MAX PLANCK INSTITUTE FOR THE PHYSICS OF COMPLEX SYSTEMS
Dresden, Germany, Sept.2010
Intern

- Worked on the development of mathematical models for DNA-based quantum computers
- Developed non-linear dynamical system model
- Wrote an article on Klein-Gordon equation solver for split-ring resonator metamaterials
- Applied non-linear dynamical model for resonator metamaterials

CENTRAL GLASS AND CERAMIC RESEARCH INSTITUTE
Kolkata, India, June 2010 – July 2010
Intern

- Worked on experimental and modelling of nanoindentation of carbon fiber-reinforced hydroxyapatatite
- Performed finite element simulations for nanoindentation
- Carried out atomic force-microscopy (AFM) experiments

COURSES

Multiscale Modeling and Simulation of Mechanical Systems - 535.737
AI for Materials - EN.510.463/663
Applied Quantum Computing – EN.520.677

AWARDS

NIST MML Accolade 2017, "For exceptional contributions in the field of data computing and data sharing for materials discovery including designing and populating two new data repositories for ab-initio and classically-computed material properties".
American Physical Society Fellow 2025, "For foundational contributions to data-driven materials discovery, including the creation of JARVIS infrastructure and machine learning tools integrating classical, quantum, and AI methods to accelerate computational and experimental materials research."
Top 2% scientist, 2025 Rank 27042

PUBLICATIONS

Google-scholar page: https://scholar.google.com/citations?user=klhV2BIAAAAJ&hl=en
H-index: **47**,
Number of citations: **9554**

Journal Articles and Preprints

1. JD Kunz, **K. Choudhary**, Mesh Graph Neural Network Framework for Accelerating Finite Element Simulation for Arbitrary Geometries, arXiv:2606.08287 (2026).

2. FM Abel, J Lee, CR Campbell, **K. Choudhary**, RamanGPT: Bidirectional Mapping Between Crystal Structures and Raman Spectra with Graph Neural Networks and Generative Transformers, arXiv:2606.03764 (2026).
3. Y Li, D Wines, **K. Choudhary**, V Gupta, MNT Kilic, S Chakrabarty, et al., Determinism analysis in Hybrid-LLM-GNN modeling for materials property prediction, Machine Learning: Science and Technology 7 (3), 035031 (2026).
4. JA Warren, F Tavazza, A McDannald, AG Kusne, H Joress, **K. Choudhary**, et al., Overcoming Roadblocks for Implementing AI/ML Methods for Materials Advancement, Annual Review of Materials Research 56 (2026).
5. V Biryukov, **K. Choudhary**, T Bazhirov, AI-ready design of realistic 2D materials and interfaces with Mat3ra-2D, arXiv:2603.27886 (2026).
6. B Slautin, K Barakati, U Pratiush, **K. Choudhary**, et al., From Photons to Electrons: Accelerated Materials Discovery via Random Libraries and Automated Scanning Transmission Electron Microscopy, arXiv:2603.20858 (2026).
7. V Dovale-Farelo, P Tavadze, MAL Marques, S Das, **K. Choudhary**, et al., System-conditioned reparameterization of the SCAN functional for accurate bandgaps: from analytical constraints to machine learning, npj Computational Materials (2026).
8. V Dovale-Farelo, **K. Choudhary**, Effect of Exchange-Correlation Functionals on Schottky Barriers at Si/Metal Interfaces, The Journal of Physical Chemistry C (2026).
9. V Gupta, **K. Choudhary**, Y Li, MNT Kilic, D Wines, W Liao, A Choudhary, et al., Dynamic embedding representation for graph neural networks to enhance materials property prediction with limited datasets, Materials Research Express 13 (6), 066502 (2026).
10. V Biryukov, **K. Choudhary**, T Bazhirov, M-code: Materials categorization via ontology, dimensionality and evolution, arXiv:2602.14384 (2026).
11. H Xin, JR Kitchin, N López, NM Schweitzer, M Abolhasani, N Artrith, **K. Choudhary**, et al., Transparent Reporting for Agentic Catalysis Enabled by Artificial Intelligence (TRACE-AI): Community Guidelines and A Publication Checklist (2026).
12. J Lee, H Neralla, CR Campbell, K Zhang, A Ajith, J Ely, **K. Choudhary**, et al., Lessons Learned from the 2025 Agentic AI for Science Hackathon (2026).
13. Muhammed Nur Talha Kilic, Daniel Wines, **Kamal Choudhary**, Vishu Gupta, Youjia Li, Sayak Chakrabarty, Wei-Keng Liao, Alok Choudhary, Ankit Agrawal, Evaluating large language models for inverse semiconductor design, Digital Discovery (2026).
14. IJ Park, **K Choudhary**, CHIPS-TB: Evaluating Tight-Binding Models For Metals, Semiconductors, and Insulators, The Journal of Physical Chemistry C 130 (7), 2814-2824 (2026).
15. **K. Choudhary**, SlaKoNet: A Unified Slater-Koster Tight-Binding Framework Using Neural Network Infrastructure for the Periodic Table, J. Phys. Chem. Lett. 16, 11109 (2025).
16. **K. Choudhary**, The JARVIS infrastructure is all you need for materials design, Computational Materials Science 259, 114063 (2025).
17. **K. Choudhary**, ChatGPT Material Explorer: Design and Implementation of a Custom GPT Assistant for Materials Science Applications, Integrating Materials and Manufacturing Innovation, 1-8 (2025)
18. **K. Choudhary**, MicroscopyGPT: Generating Atomic-Structure Captions from Microscopy Images of 2D Materials with Vision-Language Transformers, Journal of Physical Chemistry Letters 16, 7028 (2025)
19. **K. Choudhary**, DiffractGPT: Atomic Structure Determination from X-ray Diffraction Patterns Using a Generative Pretrained Transformer, Journal of Physical Chemistry Letters 16, 2110-2119 (2025).

20. FM Abel, P Burke, D Wines, B Donovan, ME Jamer, **K Choudhary**, Machine Learning for Predicting Magnetization from X-ray Diffraction of Iron Oxide Nanoparticles Using Simple Physics-Based Data Generation, arXiv:2512.13909 (2025).
21. Sayak Chakrabarty, **Kamal Choudhary**, Daniel Wines, Youjia Li, Vishu Gupta, Muhammed Nur Talha Kilic, Alok Choudhary, Ankit Agrawal, Predicting Lattice Parameters from Atomic-Scale Images of Two Dimensional Materials Using Deep Learning, J. Phys. Chem. C (2025).
22. J Lee, J Ely, K Zhang, A Ajith, CR Campbell, **K Choudhary**, AGAPI-Agents: An Open-Access Agentic AI Platform for Accelerated Materials Design on AtomGPT. Org, arXiv:2512.11935 (2025).
23. CR Campbell, AH Romero, **K Choudhary**, AtomBench: A Benchmark for Generative Atomic Structure Models using GPT, Diffusion, and Flow Architectures, arXiv:2510.16165 (2025).
24. N Pollard, **K Choudhary**, Benchqc: A benchmarking toolkit for quantum computation, Journal of computational chemistry 46 (21), e70202 (2025).
25. X Jiang, H Sun, **K Choudhary**, H Zhuang, Q Nian, Interpretable ensemble learning for materials property prediction with classical interatomic potentials, Nature: npj Computational Materials 11 (1), 319 (2025).
26. C Ginter, **K Choudhary**, S Mandal, Accelerated prediction of dielectric functions in solar cell materials with graph neural networks, arXiv:2510.08738 (2025).
27. D Wines, **K Choudhary**, Chips-ff: Evaluating universal machine learning force fields for material properties, ACS Materials Letters 7 (6), 2105-2114 (2025).
28. C Campbell, A Romero, **K Choudhary**, AtomBench: A Benchmark for Generative Atomic Structure Models using GPT, Diffusion, and Flow Architectures, arXiv 2510.16165 (2025).
29. N Pollard, **K Choudhary**, Benchqc: A benchmarking toolkit for quantum computation, Journal of Computational Chemistry 46 (21), e70202 (2025)
30. SH Wang, H Xin, L Achenie, **K Choudhary**, Examining Generalizability of AI Models for Catalysis, Journal of Catalysis, 116171 (2025).
31. Cristiano Malica, Kostya S Novoselov, Amanda S Barnard, Sergei V Kalinin, Steven R Spurgeon, Karsten Reuter, Maite Alducin, Volker L Deringer, Gábor Csányi, Nicola Marzari, Shirong Huang, Gianaurelio Cuniberti, Qiushi Deng, Pablo Ordejón, Ivan Cole, **Kamal Choudhary**, Kedar Hippalgaonkar, Ruiming Zhu, O Anatole von Lilienfeld, Mohamed Hibat-Allah, Juan Carrasquilla, Giulia Cisotto, Alberto Zancanaro, Wolfgang Wenzel, Andrea C Ferrari, Andrey Ustyuzhanin, Stephan Roche, Artificial intelligence for advanced functional materials: exploring current and future directions, J. Phys. Mater. 8 021001 (2025).
32. Daniel Wines, Akram Ibrahim, Nishwanth Gudibandla, Tehseen Adel, Frank M Abel, Sharadh Jois, Kayahan Saritas, Jaron T Krogel, Li Yin, Tom Berlijn, Aubrey T Hanbicki, Gregory M Stephen, Adam L Friedman, Sergiy Krylyuk, Albert Davydov, Brian Donovan, Michelle E Jamer, Angela R Hight Walker, **Kamal Choudhary**, Francesca Tavazza, Can Ataca , A combined Quantum Monte Carlo and DFT study of the strain response and magnetic properties of two-dimensional (2D) 1T-VSe with charge density wave, ACS nano 19 (10), 9925-9935 (2025).
33. P Ray, **K Choudhary**, SR Kalidindi, Lean CNNs for mapping electron charge density fields to material properties, Integrating Materials and Manufacturing Innovation 14 (1), 1-13 (2025).
34. A McDannald, DW Siderius, B DeCost, **K Choudhary**, DL Ortiz-Montalvo, Intrinsic Direct Air Capture, arXiv:2501.04825 (2025).
35. Ryan Jacobs, Dane Morgan, Siamak Attarian, Jun Meng, Chen Shen, Zhenghao Wu, Clare Yijia Xie, Julia H Yang, Nongnuch Artrith, Ben Blaiszik, Gerbrand Ceder, **Kamal Choudhary**, Gabor Csanyi, Ekin Dogus Cubuk, Bowen Deng, Ralf Drautz, Xiang Fu, Jonathan Godwin, Vasant Honavar, Olexandr Isayev, Anders Johansson, Stefano Martiniani, Shyue Ping Ong, Igor

Poltavsky, KJ Schmidt, So Takamoto, Aidan P Thompson, Julia Westermayr, Brandon M Wood, Boris Kozinsky , A practical guide to machine learning interatomic potentials–Status and future, Current Opinion in Solid State and Materials Science, 35, 101214 (2025).

36. **K. Choudhary**, AtomGPT: Atomistic Generative Pre-trained Transformer for Forward and Inverse Materials Design, Journal of Physical Chemistry Letters 15 (27), 6909 (2024).
37. **K Choudhary**, SLMat: A Comprehensive Serverless Toolkit for Advanced Materials Design, ChemArxiv (2024).
38. **K. Choudhary** et al., Large Scale Benchmark of Materials Design Methods, npj Computational Materials 10 (1), 93 (2024).
39. N Pollard, **K Choudhary**, BenchQC: A Benchmarking Toolkit for Quantum Computation , arXiv:2502.09595 (2024).
40. L Lang, E Hernandez, **K Choudhary**, AH Romero, ParquetDB: A Lightweight Python Parquet-Based Database, arXiv:2502.05311 (2024).
41. P Ray, **K Choudhary**, SR Kalidindi, Lean CNNs for Mapping Electron Charge Density Fields to Material Properties, Integrating Materials and Manufacturing Innovation, 1-13 (2024).
42. Y Huang, SH Wang, LEK Achenie, **K Choudhary**, H Xin, Origin of unique electronic structures of single-atom alloys unraveled by interpretable deep learning, Journal of Chemical Physics 161 (16), 2024.
43. D Wines, **K Choudhary**, Data-driven design of high pressure hydride superconductors using DFT and deep learning, Materials futures 3 (2), 025602 (2024).
44. KT Butler, **K Choudhary**, G Csanyi, AM Ganose, SV Kalinin, D Morgan, Setting standards for data driven materials science, npj Computational Materials 10 (1), 231 (2024).
45. A McDannald, DW Siderius, B DeCost, **K Choudhary**, DL Ortiz-Montalvo, Intrinsic Direct Air Capture, arXiv:2501.04825 (2024).
46. Y Li, V Gupta, MNT Kilic, **K Choudhary**, D Wines, W Liao, A Choudhary, Hybrid-LLM-GNN: integrating large language models and graph neural networks for enhanced materials property prediction, Digital Discovery (2024).
47. Md Habibur Rahman, Prince Gollapalli, Panayotis Manganaris, Satyesh Kumar Yadav, Ghanshyam Pilania, Brian DeCost, **Kamal Choudhary**, Arun Mannodi-Kanakkithodi, Accelerating defect predictions in semiconductors using graph neural networks, APL Machine Learning, 2, 1 (2024).
48. P Minch, R Bhattarai, **K Choudhary**, TD Rhone, Predicting magnetic properties of van der Waals magnets using graph neural networks, Physical Review Materials 8 (11), 114002 (2024).
49. D Wines, **K Choudhary**, CHIPS-FF: Evaluating Universal Machine Learning Force Fields for Material Properties, arXiv:2412.10516 (2024)
50. **K. Choudhary**, B. DeCost, L. Major, K. Butler, J. Thiyagalingam, F. Tavazza, Unified graph neural network force-field for the periodic table, Digital Discovery 2 (2), 346 (2023).
51. **K. Choudhary**, R. Gurunathan, B.DeCost, A. Biacchi, Atomvision: A machine vision library for atomistic images, J. Chem. Inf. Model. 2023, 63, 6, 1708 (2023)
52. **K. Choudhary**, M. Kelly, ChemNLP: A Natural Language Processing based Library for Materials Chemistry Text Data, J. Phys. Chem. C 2023, 127, 35, 17545 (2023).
53. **K. Choudhary**, K. Garrity, Designing High-Tc Superconductors with BCS-inspired Screening, Density Functional Theory and Deep-learning, npj Computational Materials 8 (1), 244 (2023).
54. **K. Choudhary**, BG Sumpter, A Deep-learning Model for Fast Prediction of Vacancy Formation in Diverse Materials, AIP Advances 13 (9) (2023).
55. D Wines, R Gurunathan, KF Garrity, B DeCost, AJ Biacchi, F Tavazza, **K Choudhary**, Recent progress in the JARVIS infrastructure for next-generation data-driven materials design, Appl. Phys. Rev. 10, 041302 (2023).

56. D Wines, T Xie, **K Choudhary**, Inverse design of next-generation superconductors using data-driven deep generative models, J. Phys. Chem. Lett. 2023, 14, 29, 6630 (2023).
57. Imran et al., 14 examples of how LLMs can transform materials science and chemistry: a reflection on a large language model hackathon,
58. Kangming Li, Daniel Persaud, **Kamal Choudhary**, Brian DeCost, Michael Greenwood, Jason Hattrick-Simpers, Exploiting redundancy in large materials datasets for efficient machine learning with less data, Nature Communications 14, 283 (2023).
59. **K. Choudhary**, C. Chen, B. DeCost, A. Jain, F. Tavazza, R. Cohn, C.W. Park, A. Choudhary, A. Agrawal, S. Billinge, E. Holm, S. P. Ong, C. Wolverton, Recent Advances and Applications of Deep Learning Methods in Materials Science, Nature NPJ Computational Materials Science, 8, 1 (2022).
60. **K. Choudhary**, T. Yildirim, D. Siderius, A Kusne, A. McDannald, D. L Ortiz-Montalvo, Graph neural network predictions of metal organic framework CO2 adsorption properties, Computational Materials Science, 210, 111388 (2022).
61. Kangming Li, Brian DeCost, **Kamal Choudhary**, Michael Greenwood, Jason Hattrick-Simpers, A critical examination of robustness and generalizability of machine learning prediction of materials properties, arXiv:2210.13597 (2022).
62. Daniel Wines, **Kamal Choudhary**, Francesca Tavazza, A systematic DFT+U and Quantum Monte Carlo benchmark of magnetic two-dimensional (2D) CrX (X = I, Br, Cl, F), arXiv:2209.10379 (2022).
63. Austin McDannald, Howie Joress, Brian DeCost, Avery E Baumann, A Gilad Kusne, **Kamal Choudhary**, Taner Yildirim, Daniel W Siderius, Winnie Wong-Ng, Andrew J Allen, Christopher M Stafford, Diana L Ortiz-Montalvo, Reproducible sorbent materials foundry for carbon capture at scale, Cell Reports Physical Science, 10, 2022.
64. R Gurunathan, **K. Choudhary**, F Tavazza, Rapid Prediction of Phonon Structure and Properties using an Atomistic Line Graph Neural Network (ALIGNN), arXiv:2207.12510 (2022).
65. N Nguyen, SYV Louis, L Wei, **K. Choudhary**, M Hu, J Hu, Predicting Lattice Vibrational Frequencies Using Deep Graph Neural Networks, ACS Omega, 7, 30, 26641 (2022).
66. J Ojih, M Al-Fahdi, AD Rodriguez, **K. Choudhary**, M Hu, Efficiently searching extreme mechanical properties via boundless objective-free exploration and minimal first-principles calculations, npj Computational Materials 8 (1), 1-12 (2022).
67. H Ucar, D Paudyal, **K. Choudhary**, Machine learning predicted magnetic entropy change using chemical descriptors across a large compositional landscape, Computational Materials Science 209, 111414 (2022).
68. M Hasan, Y Mao, **K. Choudhary**, F Tavazza, A Choudhary, A Agrawal, Data-Driven Multi-Scale Modeling and Optimization for Elastic Properties of Cubic Microstructures, IIMI, 11 (2), 230 (2022).
69. PR Kaundinya, **K. Choudhary**, SR Kalidindi, Prediction of the electron density of states for crystalline compounds with Atomistic Line Graph Neural Networks (ALIGNN), JOM 74 (4), 1395 (2022).
70. FQ Wang, **K. Choudhary**, Y Liu, J Hu, M Hu, Large scale dataset of real space electronic charge density of cubic inorganic materials from density functional theory (DFT) calculations, Scientific Data 9 (1), 1-9 (2022).
71. **K. Choudhary**, B. DeCost Atomistic Line Graph Neural Network for Improved Materials Property Predictions, Nature NPJ Computational Materials Science, 7, 1 (2021).
72. **K. Choudhary**, Quantum computation for predicting electron and phonon properties of solids, J. Phys.: Cond. Matter 33 385501 (2021).

73. **K. Choudhary**, F. Tavazza, Predicting anomalous quantum confinement effect in van der Waals materials, Phys. Rev. Mat., 5, 054602 (2021).
74. **K. Choudhary**, K. Garrity, N. Ghimire, N Anand, F. Tavazza, High-throughput search for magnetic topological materials using spin-orbit spillage, machine learning, and experiments, Phys. Rev. B 103 (15), 155131 (2021).
75. **K. Choudhary**, K. Garrity, C. Camp, S. Kalinin, R. Vasudevan, M. Ziatdinov, F. Tavazza, Computational scanning tunneling microscope image database, Nature Sci. Data, 8, 57 (2021).
76. K. Garrity, **K. Choudhary**, Fast and Accurate Prediction of Material Properties with Three-Body Tight-Binding Model for the Periodic Table, arXiv:2112.11585 (2021).
77. V. Gupta, **K. Choudhary**, F. Tavazza, C. Campbell, W. Liao, A. Choudhary, A. Agrawal, Cross-property deep transfer learning framework for enhanced predictive analytics on small materials data, Nature communications 12 (1), 1-10 (2021).
78. V. Stanev, **K. Choudhary**, A. G. Kusne, J. Paglione, I. Takeuchi, Artificial Intelligence for Search and Discovery of Quantum Materials, Communications Materials, 2, 105 (2021).
79. C. W. Andersen et al., OPTIMADE, an API for exchanging materials data, Scientific Data, 8, 217 (2021).
80. F. Tavazza, B. DeCost, **K. Choudhary**, Uncertainty Prediction for Machine Learning Models of Material Properties, ACS omega 6 (48), 32431-32440 (2021).
81. K. Garrity, **K. Choudhary**, Database of Wannier Tight-binding Hamiltonians using High-throughput Density Functional Theory, Sci. Data, 8, 106 (2021).
82. **K. Choudhary**, J. Ansari, I. Mazin, K. Sauer, Density Functional Theory based Electric Field Gradient Database, Nature Sci Data, 7, 362 (2020).
83. **K. Choudhary**, K. Garrity, A. Reid, B. DeCost, A. Biacchi, A. Hight Walker, Z. Trautt, J. Hattrick-Simpers, A. Gilad Kusne, A. Centrone, A.Davydov, J. Jiang, R. Pachter, G. Cheon, E. Reed, A. Agrawal, X. Qian, V. Sharma, H. Zhuang, S. Kalinin, B. Sumpter, G.Pilania, P. Acar, S. Mandal, K. Haule, D. Vanderbilt, K. Rabe, F. Tavazza, The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design, Nature NPJ Computational Materials, 6, 173 (2020).
84. **K. Choudhary**, K. Garrity, F. Tavazza, Data-driven Discovery of 3D and 2D Thermoelectric Materials, J. Phys.: Cond. Matt. 32 (47), 475501(2020).
85. **K. Choudhary**, K. Garrity, V. Sharma, A. Biacchi, A. Walker, F. Tavazza, High-throughput density functional perturbation theory and machine learning predictions of infrared, piezoelectric, and dielectric responses, Nature NPJ Computational Materials, 6, 1 (2020).
86. **K. Choudhary**, K. Garrity, J. Jiang, R. Pachter, Computational search for magnetic and non-magnetic 2D topological materials using unified spin–orbit spillage screening, Nature NPJ Computational Materials, 6, 1 (2020).
87. **K Choudhary**, KF Garrity, G Pilania, F Tavazza, Efficient computational design of 2D van der Waals Heterostructures: band-alignment, lattice-mismatch, web-app generation and machine-learning, arXiv:2004.03025 (2020).
88. **K. Choudhary**, M. Bercx, J. Jiang, R. Pachter, D. Lamoen, F. Tavazza, Accelerated Discovery of Efficient Solar Cell Materials Using Quantum and Machine-Learning Methods, Chemistry of Materials, 31, 15, 5900-5908 (2019).
89. **K Choudhary**, KF Garrity, F Tavazza, High-throughput discovery of topological materials using spin-orbit spillage, Sci. Rep. 9, 8534 (2019).
90. **K. Choudhary**, F. Tavazza, Convergence and machine learning predictions of Monkhorst-Pack k-points and plane-wave cut-off in high-throughput DFT calculations, Comp. Mat. Sci. 161, 300 (2019).

91. D. Jha, **K. Choudhary**, F. Tavazza, Wei-keng Liao, A. Choudhary, C. Campbell, and A. Agrawal, Enhancing Materials Property Prediction by Leveraging Computational and Experimental Data using Deep Transfer Learning, Accepted Nature Communications (2019).
92. R. K. Vasudevan, **K. Choudhary**, A. Mehta, R. Smith, G. Kusne, F. Tavazza, L. Vlcek , M. Ziatdinov, S. V. Kalinin and J. Hattrick-Simpers, Materials science in the artificial intelligence age: high-throughput library generation, machine learning, and a pathway from correlations to the underpinning physics, MRS Communications. 1 (2019)
93. JR Hattrick-Simpers, **K. Choudhary**, C Corgnale, A simple constrained machine learning model for predicting high-pressure-hydrogen-compressor materials, Molecular Systems Design & Engineering 3 (3), 509-517 (2019).
94. Q. Zhu, T. Frolov, and **K. Choudhary**, Computational Discovery of Inorganic Electrides from an Automated Screening, Matter 1,1 (2019).
95. P Wang, MC Peters, UR Kattner, **K. Choudhary**, GB Olson, Thermodynamic analysis of the topologically close packed σ phase in the CoCr system, Intermetallics 105, 13-20 (2019).
96. JJ Gabriel, S Xie, **K Choudhary**, M Sexton, SR Phillpot, J Xue, RG Hennig, Candidate replacements for lead in CH3NH3PbI3 from first principles calculations, Computational Materials Science 155, 69-73 (2019).
97. **K. Choudhary** et al., High-throughput assessment of vacancy formation and surface energies of materials using classical force-fields, J. Phys. Cond. Matt. 30, 395901(2018).
98. **K. Choudhary**, B. DeCost, F. Tavazza, Machine learning with force-field inspired descriptors for materials: fast screening and mapping energy landscape, Phys. Rev. Mat., 2, 083801 (2018).
99. **K. Choudhary** et al., Elastic properties of bulk and low-dimensional materials using van der Waals density functional, Phys. Rev. B, 98, 014107 (2018).
100. **K. Choudhary** et al., Computational Screening of High-performance Optoelectronic Materials using OptB88vdW and TBmBJ Formalisms, Nature Scientific Data 5, 180082 (2018).
101. **K. Choudhary** et al., High-throughput Identification and Characterization of Two-dimensional Materials using Density functional theory, Nature Sci. Rep. 7, 5179 (2017).
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109. Alexandre F. Fonseca, Tao Liangb, Difan Zhang, **K. Choudhary**, Susan B. Sinnott, "Probing the accuracy of reactive and non-reactive force fields to describe physical and chemical properties of graphene-oxide", Computational Materials Science 114, 236 (2016).

110. **K. Choudhary**, Aleksandr Chernatynskiy, E. W. Bucholz, Richard Hennig, Simon Phillpot, Susan B. Sinnott "Computational Search of Lanthanide Doped and Co-doped Y3Al5O12 for Optoelectronic Applications", Appl. Phys. Lett. 107, 112109 (2015).
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117. **K. Choudhary**, L. Hill, T. Kemper, S. B. Sinnott, "Mechanisms for hyperthermal polyatomic hydrocarbon modification of PMMA surfaces from molecular dynamics simulations", J. Vac. Sci. Technol. A 31, 061403 (2013).
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SOFTWARE & DATASETS

NIST-JARVIS infrastructure (>200,000 users): jarvis.nist.gov
Open datasets: ~3 million downloads (figshare.com/authors/Kamal_Choudhary/4445539)
AtomGPT.org & ChatGPT Material Explorer (~10,000 users)
Open-access AI/ML packages (15+): github.com/atomgptlab
AGAPI, InterMat, SlaKoNet, DefectMat, AtomGPT, DiffractGPT, MicroscopyGPT, ALIGNN, ChemNLP, AtomVision, TB3Py, CHIPSFF, SLMat, BenchQC, JARVIS-Leaderboard, JARVIS-tools.

TALKS AND PRESENTATIONS

1. Gordon Research Conference, AI for Materials, Energy, and Chemical Sciences, Texas, 2026
2. Materials Research Society, Boston, 2025
3. Denver X-ray conference, Maryland, 2025
4. NCMRD, S. Korea, 2025
5. Center for AI Learning and Community-Engaged Innovation, U. Baltimore, November 2025
6. Artificial Intelligence for Materials Science Workshop, Karlsruhe Institute of Technology (KIT), September 2025.
7. American Chemical Society, 2025
8. Institute for Mathematical and Statistical Innovation, University of Chicago, April 2025 (Invited).
9. American Physical Society, Anaheim, 2025
10. AIMED workshop, Chicago, 2024
11. AI for Materials workshop, U. Barcelona, 2024
12. CNMS workshop, Oak ridge, 2024
13. IIT Chennai workshop, 2024
14. Accelerate conference, U. Toronto, 2023
15. Materials Research Society, Boston, 2023
16. Atomistic Line Graph Neural Network for Improved Property Predictions, MIT GraphEx symposium, May 2022 (Invited)
17. MLP-Safe workshop, U. Wisconsin, 2023
18. NIST-JARVIS Infrastructure to Enable Deep Learning and Quantum Computation Methods for Improved Materials Design, UK Research and Innovation, April 2022 (Invited).
19. Deep Learning and Quantum Computation Methods for Improved Materials Design, Materials project seminar series, October 13, 2021 (Invited).
20. Deep Neural Network for Improved Materials Property Predictions, IMRC MRS, August 16, 2021 (Invited).
21. Deep Neural Network for Improved Materials Property Predictions, EUSPN, June 10, 2021 (Invited).
22. High-throughput search for magnetic topological materials using spin-orbit spillage, machine-learning and experiments, NGSCES, June 10, 2021.
23. OPTIMADE API for JARVIS data, June 7, 2021 (Invited).

24. Accelerated Discovery of Efficient Solar Cell Materials Using Quantum and Machine-Learning Methods, Am. Ceramic Soc., January 19, 2021 EMA,
25. High-throughput Discovery of Topologically Non-trivial Materials using Spin-orbit Spillage, TMS, Feb 27, 2020.
26. NIST-JARVIS database, LBNL seminars, Feb. 2, 2020 (Invited).
27. Johns Hopkins University PARADIM summer school, August 2019 (Invited).
28. JARVIS Databases and Tools for High-throughput Computation and Machine-learning, University of Nevada, Las Vegas, April 19, 2019 (Invited).
29. Unified Machine-learning Models for Materials: Crystals, Surfaces, Grain-boundaries, Molecules, Proteins, U. Wyoming, April 10, 2019 (Invited).
30. Unified Machine-learning Models for Materials: Crystals, Surfaces, Molecules, Proteins, TMS, San Antonio, Mar.14, 2019.
31. Computational Database of 3D and 2D materials, TMS, San Antonio, Mar.11, 2019.
32. Database of Topological Materials & Spin-orbit Spillage, APS, Boston, Nov 30, 2018.
33. Machine learning with force-field-inspired descriptors for materials: Fast screening and mapping energy landscape, MRS, Boston, Nov 20, 2018.
34. Accelerated Materials Discovery & Characterization with Quantum and Machine learning approaches, IIT BHU, Nov. 19, 2018, (Invited).
35. Accelerated Materials Discovery & Characterization with Quantum and Machine learning approaches, PARADIM, Johns Hopkins Univ., Nov. 14, 2018, (Invited).
36. 2D/3D materials screening and genetic algorithm with ML model, AIMS workshop, August 07, 2018, NIST, Maryland, (Invited).
37. 2D/3D materials screening and genetic algorithm with ML model, August 02, 2018, University of Maryland, MLMR, 2018, (Invited).
38. Physics inspired artificial intelligence/machine learning, Google:DevFestDC, June 08, 2018, Virginia, (Invited).
39. Joint Automated Repository for Various Integrated Simulations, Mar. 19, 2018, Citrine Informatics, 2018, California, (Invited).
40. Joint Automated Repository for Various Integrated Simulations, Mar. 16, 2018, Google Inc., 2018, California, (Invited).
41. Utilizing Error in First-principle Lattice Constants to Discover Novel Low-dimensional Materials (TMS), Mar. 15, 2018, Phoenix, AZ.
42. High-throughput Evaluation and Comparison of Classical Interatomic-potentials: Structural, Elastic, Defect, Surface and Phonon Properties (TMS), Mar. 13, 2018, Phoenix, AZ.
43. Computational Screening of Novel Two-dimensional Topological Insulators and Layer-dependent Properties, TMS, Mar. 12, 2018, Phoenix, AZ.
44. Towards Efficient Optoelectronic Material Design using Density Functional Theory, Experiments and Machine Learning, Electronic and Advanced Materials (American Ceramic Society), Jan. 19, 2018, Orlando.
45. High-throughput Identification and Characterization of Two-dimensional Materials Using Density Functional Theory, Energy Materials, December 06, 2017, Dallas (Invited).
46. High-throughput Identification and Characterization of Two-dimensional Materials Using Density Functional Theory, Materials Science and Technology (MS & T), October 09, 2017.
47. Classical Force-field and Quantum Density Functional Theory Database, Applied Crystallography, October 16, 2017, Chicago (Invited).

48. High-throughput Identification and Characterization of Two-dimensional Materials Using Density Functional Theory, American Chemical Society, August 20, 2017, Washington D.C.
49. Computational Discovery of Two-Dimensional Materials, Society for Industrial and Applied Mathematics (SIAM), July 12, 2017, Pittsburg, Pennsylvania (Invited).
50. High-throughput Identification and Characterization of Two-dimensional Materials Using Density Functional Theory, Annual Workshop on Recent Developments in Electronic Structure Methods, Poster presentation, June 25, 2017, Princeton University, Princeton, New Jersey.
51. High-throughput Identification and Characterization of Two-dimensional Materials using Density functional theory, Graphene and Beyond, May 9-12, 2017, Penn State University, Pennsylvania.
52. Computational Discovery of Two-Dimensional Materials, Evaluation of Force-Fields and Machine Learning, Integrated Computational Materials Engineering, May 24, 2017, Ypsilanti, Michigan.
53. Computational Discovery of Two-Dimensional Materials, Evaluation of Force-Fields and Machine Learning, Northwestern University, CHIMAD Seminar, May 19, 2017, Evanston, Illinois (Invited).
54. Structural and Vibrational Properties of MoTe2 Polymorph and JARVIS database, The Minerals, Metals & Materials Society (TMS), March 1, 2017, San Diego, California.
55. Evaluation and comparison of classical interatomic potentials through a user-friendly interactive web-interface, The Minerals, Metals & Materials Society (TMS), March 1, 2017, San Diego, California.
56. High-throughput Characterization of Materials using Molecular-Dynamics and Density functional theory, March 21, 2017, Wright State University and Air-force research lab (AFRL), HPC Enabled Data Analytics Workshop, Dayton, Ohio (Invited)
57. Computational Discovery of Two-Dimensional Materials, Evaluation of Force-Fields and Machine Learning, Group Seminar, Kieron Burke, Feb 28, 2017, University of California, Irvine. (Invited)
58. High-throughput Density Functional Theory for Optoelectronic Materials, Evaluation of Force-Fields and Machine Learning, NIST Baglunch Seminar, Feb 22, 2017, Gaithersburg, Maryland. (Invited)
59. Evaluation and comparison of classical interatomic potentials through a user-friendly interactive web-interface, LAMMPS tutorial and Materials Simulation Symposium, August 15-19, 2016, Temple University, Philadelphia, Pennsylvania.
60. Evaluation and comparison of classical interatomic potentials through a user-friendly interactive web-interface, NIST Sigma Xi poster presentation, April 20, 2016, NIST, Gaithersburg, Maryland.

PROFESSIONAL SERVICE & LEADERSHIP

Associate Editor: npj Computational Materials (Nature Portfolio)
Editorial team: Materials Today Communications, PRX Energy, Scientific Data
Founder & CEO: DeepMaterials LLC
Organizer: AI for Materials Science (AIMS), Quantum Matters in Materials Science (QMMS) workshops, JARVIS-School tutorials
Member: TMS, APS, MRS

MENTORSHIP

Mentored 6 postdoctoral researchers and 9 Ph.D. students.

OUTREACH & SCIENCE COMMUNICATION

AtomGPT Lab YouTube channel: youtube.com/@dr_k_choudhary
"50 Apps in 50 Days": daily materials-AI app series on LinkedIn / X
7-hour recorded lecture series on materials AI/ML (YouTube)
Organizer / co-organizer of community events: AI for Materials Science (AIMS), Quantum Matters in Materials Science (QMMS), AI4Science, and Microscopy hackathons.