Avanish Mishra, Ph.D.

Personal Data

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Summary of Qualifications

- Computational materials scientist with 8+ years of experience in density functional theory, molecular dynamics, materials physics and chemistry, and machine learning
- Authored 20+ publications in peer-reviewed journals, including 2 review articles
- Co-developed computational materials database, "aNANt" (http://anant.mrc.iisc.ac.in/)
- Build and utilized virtual characterization tools (texture and diffraction analyses)

Current Positions

Oct 2022-Present	Director's Postdoctoral Fellow, **Theoretical Division (T-1), Physics and Chemistry of Materials, Los Alamos National Laboratory**, Los Alamos, NM, USA

Education

Aug 2014-Feb 2019	PhD in Science, **Materials Research Centre, Indian Institute of Science**, Bengaluru, India
CGPA: 7.3/8.0	**Advisor:** Prof. Abhishek Kumar Singh **Dissertation:** Exploration of exfoliation, functionalization and properties of MXenes via first-principles and machine learning
July 2013	Master of Science in Physics
Marks: 920/1200	**Deen Dayal Upadhyaya Gorakhpur University**, Gorakhpur, India
July 2011	Bachelor of Science in Physics, Math, and Chemistry
Marks: 1152/1800	**Deen Dayal Upadhyaya Gorakhpur University**, Gorakhpur, India

Research experience

Director's Postdoctoral Fellow	Los Alamos National Laboratory, Los Alamos, NM, USA
Oct 2022-Present	Sponsors: Dr. Edward M. Kober and Dr. Nithin Mathew

Grain boundary characterization from diffractograms by physics-informed machine learning

- Identified Grain boundary motifs using Graph theory and strain functional descriptors
- Explored role of local atomic structure in controlling dislocation-grain boundary reaction using machine learning
- Simulated synchrotron X-ray diffraction to expedite grain boundary characterization from experimental diffractograms by using physics-informed neural networks

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Postdoctoral Fellow | Los Alamos National Laboratory, Los Alamos, NM, USA
Jan 2022-Sep 2022 | Mentors: Dr. Edward M. Kober and Dr. Nithin Mathew

Microstructure characterization using atomistic simulations and machine learning

- Used machine learning algorithms for automated analysis of atomistic simulation data and up-scaling to mesoscale models
- Identified physically meaningful atomic environment at Grain boundaries using strain functional descriptors and unsupervised learning
- Established Structure-property relationship for grain boundary energy and atomic energy density using supervised machine learning

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Research Scientist | University of Connecticut, Storrs, CT, USA
May 2021-Dec 2021 | Mentor: Prof. Avinash M. Dongare

Investigating the links between microstructure and the atomic scale behavior of metals under dynamic loading conditions

- Developed an on-the-fly tool (VirTex) for orientation mapping to identify twinning and phase variants, and Slip systems from atomistic simulations
- Extended the application of virtual X-ray diffraction and texture methods to mesoscale (Quasi-Coarse-Grained Dynamics)
- Mentored and contributed to accelerated data-driven discovery of promising layered materials for energy storage
- Mentored and contributed to develop an interatomic potential to model shock deformation of various Cu/Mo interface microstructure

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Postdoctoral Fellow | University of Connecticut, Storrs, CT, USA
May 2019-April 2021 | Mentor: Prof. Avinash M. Dongare

Investigating the links between microstructure and the atomic scale behavior of multiphase metallic materials under dynamic loading conditions

- Constructed an interatomic potential to model pressure dependent phase transformation in Fe of various Cu/Fe interface microstructure
- Fingerprinted prominent deformation modes in metals using virtual X-ray diffraction (XRD) and Selected area electron diffraction (SAED) patterns
- Identified stable phases of Fe clusters in Cu matrix, and Cu clusters in Fe matrix under high-strain rate deformation
- Mentored and contributed in investigating lithiation driven phase transformation and formation of local heterostructures in transition metal chalcogenides

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Graduate Researcher | Indian Institute of Science, Bengaluru, KA, India
Aug 2014-Feb 2019 | Advisor: Prof. Abhishek Kumar Singh

Exploration of exfoliation, functionalization and properties of MXenes via first-principles and machine learning

- Proposed possible route for exfoliating the pristine MXenes and explored thermodynamics of non-uniform and random functionalization
- Performed thousands of density functional theory calculations to develop India's first computation materials database, "aNANt"
- Trained machine learning model to predict high-accuracy GW band gap and edges of MXenes for identifying promising photo-catalytic material
- Proposed a new feature selection approach (Feature blending) to develop generalized machine learning models for property prediction
- Investigated stable phases of oxygen-functionalized MXenes, and predicted highest reported out-of-plane polarization in layered materials

Publications

Total **1066 citations and h-index of 11** (source: Google scholar at March 10, 2023)

Peer-reviewed articles:

1. **A. Mishra**, P. Srivastava, H. Mizuseki, K-R. Lee and Abhishek K. Singh, "*Isolation of pristine MXene from Nb_4AlC_3 MAX phase: A first-principles Study*" **Phys. Chem. Chem. Phys. 18, 11073 (2016)**

2. P. Srivastava*, **A. Mishra***, H. Mizuseki, K-R. Lee and Abhishek K. Singh, "*Mechanistic Insight into the Chemical Exfoliation and Functionalization of Ti_3C_2 MXene*", **ACS Appl. Mater. Interfaces. 8, 24256 (2016)** | *Equal contribution

3. **A. Mishra**, P. Srivastava, A. Carreras, I. Tanaka, H. Mizuseki, K-R. Lee and Abhishek K. Singh,, "*Atomistic Origin of Phase Stability in Oxygen Functionalized MXene: A Comparative Study*", **J. Phys. Chem. C 121, 18947 (2017)**

4. A. Chandrasekaran, **A. Mishra**, and Abhishek K. Singh, "*Ferroelectricity, Antiferroelectricity, and Ultrathin 2D Electron/Hole Gas in Multifunctional Monolayer MXene*", **Nano Lett., 17, 3290 (2017)**

5. R. Koizumi, S.Ozden, A. Samanta, A. P. P. Alves, **A. Mishra**, G. Ye, G. G. Silva, R. Vajtai, Abhishek K. Singh, C. S. Tiwary, and P M. Ajayan, "*Origami-Inspired 3D Interconnected Molybdenum Carbide Nanoflakes*" **Adv. Mater. Interfaces 5, 1701113 (2018)**

6. A. C. Rajan*, **A. Mishra***, S. Satsangi, R. Vaish, H. Mizuseki, K-R. Lee and Abhishek K. Singh, "*Machine-Learning-Assisted Accurate Band Gap Predictions of Functionalized MXene.* **Chem. Mater 30, 4031 (2018)** | *Equal contribution

   -Mentioned as seminal article in Virtual Issue on Machine-Learning Discoveries in Materials Science of Chemistry of Materials

7. **A. Mishra***, S. Satsangi*, A. C. Rajan, H. Mizuseki, K-R. Lee and Abhishek K. Singh, *"Accelerated Data-Driven Accurate Positioning of the Band-Edges of MXenes."* **J. Phys. Chem. Lett. 10, 780 (2019)** | *Equal contribution

8. M. Khazaei, **A. Mishra**, N. S. Venkataramanan, Abhishek K. Singh and S. Yunok, *"Recent Advances in MXenes: From Fundamentals to Applications."* **Curr. Opin. Solid State Mater. Sci. 23, 164 (2019)**

9. N. Sethulakshmi, **A. Mishra**, P. M. Ajayan, Y. Kawazoe, A. Roy, Abhishek K. Singh and C. S. Tiwary, *"Magnetism in Two-Dimensional Materials Beyond Graphene."* **Mater. Today 27, 107 (2019)**

10. N. Lertcumfu, Farheen N. Sayed, Sharmila N. Shirodkar, S. Radhakrishnana, **A. Mishra**, G. Rujijanagul, Abhishek K. Singh, Boris. I. Yakobson, C. S. Tiwary, and P. M. Ajayan *"Structure-Dependent Electrical and Magnetic Properties of Iron Oxide Composites."* **Physica Status Solidi (A) 1801004, (2019)**

11. T. Pandey, A. Nissimagoudar, **A. Mishra** and Abhishek K. Singh, *"Ultralow Thermal Conductivity and Anomalously High Thermoelectric Figure of Merit in Ternary In_5X_5Br (X = S, and Se) Compounds."* **J. Mater. Chem. A 8, 13812 (2020)**

12. S. Parida, **A. Mishra**, J. Chen, J. Wang, C. B. Carter, and Avinash M. Dongare, *"Vertically Stacked 2H-1T Dual-phase MoS_2 Microstructures During Lithium Intercalation: A first Principles Study"* **J. Am. Ceram. Soc 103, 6603 (2020)**

13. S. N. Shuvo, A. M. U. Gomez, **A. Mishra**, W. Y. Chen, Avinash M. Dongare, and L. A Stanciu, *"Sulfur-doped Titanium Carbide MXenes for Room Temperature Gas Sensing"* **ACS Sens. 5, 2915 (2020)**

14. P. Xu, W. Rheinheimer, **A. Mishra**, S. N. Shuvo, Z. Qi, H. Wang, Avinash M. Dongare, and L. A Stanciu, *"Origin of High Interfacial Resistance in Solid-State Batteries: LLTO/LCO Half-cells"* **ChemElectroChem 8, 1847 (2021)**

15. **A. Mishra**, C. Kunka, M. J. Echeverria, R. Dingreville, and Avinash M. Dongare, *"Fingerprinting Shock-induced Deformations via Diffraction."* **Sci. Rep. 11, 9872 (2021)**

16. M. J. Echeverria, S. Galitskiy, **A. Mishra**, and Avinash M. Dongare, *"Modeling the Evolution of Microstructure during Laser Shock Loading and Spall Failure of Cu Microstructures at the Atomic Scales "* **Comput. Mater. Sci. 198, 110668 (2021)**

17. **A. Mishra**, J. Lind, M. Kumar, and Avinash M. Dongare, *"Understanding the Phase Transformation Mechanisms that affect the Dynamic Response of Fe-based Microstructures at the Atomic Scales"* **JAP 130, 215902 (2021)**

18. S. Satsangi*, **A. Mishra***, and Abhishek K. Singh, *"Feature Blending: An Approach Towards Unified Machine Learning Models for Band Gap Prediction."* **ACS Phys. Chem. Au 2, 16 (2022)** | *Equal contribution

19. **A. Mishra**, M. J. Echeverria, K. Ma, S. Parida, C. Chen, S. Galitskiy, and Avinash M. Dongare, *"Virtual Texture Analysis to Investigate the Deformation Mechanisms in Metal Microstructures at the Atomic-Scale"* **J. Mater. Sci. 57, 10549 (2022)**

    -Graphical abstract selected as cover art

20. **A. Mishra**, K. Ma, and Avinash M. Dongare, *"Virtual Diffraction Simulations using the Quasi-Coarse-Grained Dynamics Method to Understand and Interpret Plasticity Contributions during In Situ Shock Experiments"* **J. Mater. Sci. 57, 12782 (2022)**

21. C. Ching, S. Galitskiy, **A. Mishra**, and Avinash M. Dongare, *"Modeling Laser Interactions with Aluminum and Tantalum Targets using a Hybrid Atomistic-Continuum Model"* **JAP 133, 105901 (2023)**

Upcoming journal articles:

1. R. Kumar, J. Chen, **A. Mishra**, and Avinash M. Dongare, *"Interface Microstructure Effects on Dynamic Failure Behavior of Layered FCC/BCC Microstructures"* **Sci. Rep (Review received)**

2. S. Galitskiy, **A. Mishra**, and Avinash M. Dongare, *"Modeling Shock-induced Void Collapse in Single-crystal Ta Systems at the Mesoscales"* **JAP (Under Review)**

3. **A. Mishra**, S. Suresh, S. J. Fensin, E. M. Kober, and N. Mathew, *"Learning Properties of Arbitrary Grain Boundaries from Metastable Structures of Symmetric-tilts"* **LA-UR-22-32270 (Prepared for: Phys. Rev. Mater.) | (Draft available upon request)**

4. **A. Mishra**, K. Dang, S. J. Fensin, E. M. Kober, and N. Mathew, *"Role of Microscopic Degrees of Freedom on Nanopillar Compression of Bicrystal Cu"* **LA-UR-23-20212 (Prepared for: Scr. Mater.) | (Draft available upon request)**

5. S. Parida, **A. Mishra**, C. B. Carter, and Avinash M. Dongare, *"Machine Learning Assisted Search of Promising 2D-materials for Energy Application."* **(Under preparation)**

Teaching experience

Teaching assistant Aug-Dec 2015	MR 301: Quantum Mechanical Principles in Materials. Course instructor: Prof. Abhishek Kumar Singh Indian Institute of Science
Teaching assistant Jan-May 2016	MR 308: Computational modeling of materials. Course instructor: Prof. Abhishek Kumar Singh Indian Institute of Science

co-Instructor Sep-Dec 2021	MSE 6401: Graduate Seminars Materials Science and Engineering University of Connecticut

Outreach activities

Symposium Organizer April 2022	Mach Conference 2022 Co-organizer of three-day symposium titled Real-time characterization of materials under dynamic deformation
Theoretical Division May 2022 -Present	P/T (Physics/Theory) Colloquium Committee Member from Theoretical Division for P/T Colloquium

Computational Skills

Programming:	Python, Fortran, C, Git, Matlab, Bash
Materials libraries:	aNANt, pymatgen, OQMD, CMR, JARVIS, OpenKIM
Machine learning libraries:	Scikit, PyToch, tensorflow, BayesOpt
Software packages:	Vasp, LAMMPS, Quantum Espresso, Gaussian, Phonopy

Code Development

VirTex: A python package for virtual texture analysis; orientation relationship, misorientation, Schmid factor, twin characterization, (methodology and code)

Scholarships and Awards

1. **Fellowship** from Los Alamos National Laboratory (LANL), USA, to carry-out research as Director's postdoctoral fellow at LANL, USA, **Aug 2022**
2. **Travel award** from department of science and technology, India to attend American Physical Society March Meeting, USA, **Feb 2019**
3. **Travel award** from Group on Energy Research and Applications (GERA) to attend American Physical Society March Meeting, USA, **Feb 2019**
4. **Travel award** to attend MATERIALS 4.0 workshop at Technical University of Dresden, Dresden, Germany, **Sep 2018**
5. **Travel award** from Group on Energy Research and Applications (GERA) to attend American Physical Society March Meeting, USA, **Feb 2018**
6. **Travel award** to attend advance workshop at International Centre for Theoretical Physics, Trieste, Italy, **Jan 2017**
7. **Kawazoe Prize, Best poster award** in ACCMS-TM 2016 at SRM University Chennai, India, **Sep 2016**
8. **Qualified joint CSIR-UGC National Eligibility Test (NET)** 2013 (December) with all India rank of **58** in Physical Science.

9. **Qualified Graduate Aptitude Test in Engineering (GATE)** 2014 with all India rank of **36** in Physical Science.

Proposals

1. Grain Boundary Characterization from Diffractograms by Physics-informed Machine Learning (PI, HPC resources: 1 million CPU hours and 1 million GPU hours)
2. Designing Resilient and Innovative Engineering Materials for Nuclear Reactors (co-I, LDRD-DR for FY2024) | **Invited to submit an LDRD-DR Full Proposal*
3. Discover High Entropy Alloys for Extreme Thermal Conditions (co-I, DE-FOA-0002905 for FY2024) | **Encouraged for Full Proposal submission*
4. Multi-Objective Optimization Framework for High-Entropy Alloy Design (co-PI, LDRD-ER for FY2024)
5. Accelerating Scalable Manufacturing of Resilient Nanocrystalline Steels for Next-Generation Nuclear Reactors (co-I, LANL-LAB 23-3010 for FY2024)

Reviewer of Journals

- Physical Review Letters, Physical Review B, npj Computational Materials, Scientific Report, Advanced Functional Materials, Journal of Applied Physics, Journal of Materials Science, Sensors, Modelling and Simulation in Materials Science and Engineering, Computational Materials Science, and Materials

Presentations

Invited presentation

Feb 2021 "*Understanding Plasticity Contributions from Slip, Twinning, and Phase Transformation under Shock Loading using Atomistic Simulations*" **A. Mishra**, *Department of Materials Science and Engineering*, University of Connecticut, Connecticut, USA.

Oral presentation

Dec 2022 "*Structure-Property Relationships for Grain Boundaries Using Strain Functional Descriptors and Supervised Machine Learning*" **A. Mishra**, S. Suresh, K. Dang, S. J. Fensin, E. M. Kober, and N. Mathew, *2012 MRS Fall Meeting*, Hynes Convention Center, Boston, Massachusetts, USA.

Dec 2022 "*Analysis of Grain Boundary (GB) Structure and Dislocation-GB Interactions Using Unsupervised Machine Learning*" N. Mathew, **A. Mishra**, S. Suresh, K. Dang, S. J. Fensin, and E. M. Kober, *2012 MRS Fall Meeting*, Hynes Convention Center, Boston, Massachusetts, USA.

Oct 2022 *"Accurate prediction of grain boundary properties using machine learning and strain functional descriptors"* **A. Mishra**, S. Suresh, K. Dang, S. J. Fensin, E. M. Kober, and N. Mathew, *2022 SES Annual Meeting*.

April 2022 *"Real-time characterization of phase and twin variants in dynamically deformed microstructures"* **A. Mishra**, K. Ma, and Avinash M. Dongare, *2022 Mach Conference*.

Mar 2021 *"Fingerprinting Shock-Induced Deformations via Diffraction"* **A. Mishra**, C. Kunka, M. J. Echeverria, R. Dingreville, and Avinash M. Dongare, *2021 TMS Annual Meeting*.

Feb 2020 *"Slip, Twinning and Phase Transformations in Multiphase Metallic Materials under Shock Loading Conditions"* **A. Mishra**, and Avinash M. Dongare, *2020 TMS Annual Meeting*, San Diego Convention Center in San Diego, California, USA.

Mar 2019 *"Atomistic Origin of Phase Stability in Oxygen Functionalized MXene"* **A. Mishra**, P. Srivastava, A. Carreras, I. Tanaka, H. Mizuseki, K-R. Lee and Abhishek K. Singh, *2019 APS March Meeting*, Boston Convention and Center in Boston, Massachusetts, USA.

Dec 2017 *"Atomistic Origin of Phase Stability in Oxygen Functionalized MXene"* **A. Mishra**, P. Srivastava, A. Carreras, I. Tanaka, H. Mizuseki, K-R. Lee and Abhishek K. Singh, *12^{th} ACCMS VO*, Tohoku University, Sendai, Miyagi, Japan.

Dec 2017 *"Ferroelectricity, Antiferroelectricity, and Ultrathin 2D Electron/Hole Gas in Multifunctional Monolayer MXene"* A. Chandrasekaran, **A. Mishra**, and Abhishek K. Singh, *2017 MRS Fall Meeting*, Hynes Convention Center, Boston, Massachusetts, USA.

Poster presentation

Dec 2019 *"Effect of Deformation Twinning and Phase Transformation on Spall Failure of Fe"* **A. Mishra**, and Avinash M. Dongare, *2019 MRS Fall Meeting*, Hynes Convention Center, Boston, Massachusetts, USA.

Dec 2019 *"Data-Driven Accurate Positioning of the Band Edges of MXenes"* **A. Mishra**, Arunkumar C. Rajan, R. Juneja and Abhishek K. Singh, *2019 MRS Fall Meeting*, Hynes Convention Center, Boston, Massachusetts, USA.

Sep 2018 *"An Accelerated Metal-Semiconductor Classification of Functionalized MXene using Machine Learning"* **A. Mishra**, and Abhishek K. Singh, *Deep Materials: Perspectives on Data-driven Materials Research*, Technical University of Dresden, Dresden, Germany.

Feb 2018 "*Ferroelectricity, Antiferroelectricity, and Ultrathin 2D Electron/Hole Gas in Multifunctional Monolayer MXene*" A. Chandrasekaran, **A. Mishra**, and Abhishek K. Singh, *2018 Recent Advances in Molecular Simulations*, Indian Institute of Science, Bengaluru, India.

Dec 2017 "*Mechanistic Insight into the Chemical Exfoliation and Functionalization of Ti_3C_2 MXene*" P. Srivastava*, **A. Mishra***, H. Mizuseki, K-R. Lee and Abhishek K. Singh, *2017 MRS Fall Meeting*, Hynes Convention Center, Boston, Massachusetts, USA.

Jan 2017 "*Mechanistic Insight into the Chemical Exfoliation and Functionalization of Ti_3C_2 MXene*" P. Srivastava*, **A. Mishra***, H. Mizuseki, K-R. Lee and Abhishek K. Singh, *Advanced Workshop on High-Performance & High-Throughput Materials Simulations using QUANTUM ESPRESSO*, International Centre for Theoretical Physics, Trieste, Italy.

Sep 2016 "*Mechanistic Insight into the Chemical Exfoliation and Functionalization of Ti_3C_2 MXene*" P. Srivastava*, **A. Mishra***, H. Mizuseki, K-R. Lee and Abhishek K. Singh, *ACCMS-TM 2016*, SRM University, Chennai, India.

June 2016 "*Isolation of pristine MXene from Nb_4AlC_3 MAX phase: A first-principles study*" **A. Mishra**, P. Srivastava, H. Mizuseki, K-R. Lee and Abhishek K. Singh, *ICMR 2016*, Indian Institute of Science, Bengaluru, India.

References

Dr. Nithin Mathew | Staff Scientist (Postdoctoral mentor)
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