Payal Chaudhary
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EDUCATION

- University of Nebraska-Lincoln (UNL), Department of Chemical and Biomolecular Engineering, Lincoln, NE, USA, **PhD Student** — 2021-present
- IIT (BHU) Varanasi, School of Materials Science and Technology, Varanasi, India — 2014-2019
  Integrated Dual Degree (B.Tech. + M.Tech.) in Materials Science and Technology

RESEARCH EXPERIENCE

Research Assistant, Department of Chemical and Biomolecular Engineering, University of Nebraska-Lincoln — 2021-present
Advisor, Vitaly Alexandrov, PhD

- Theoretical investigation of super-Nernstian behavior in water splitting electrocatalysts using density-functional-theory based methods.
- Computational study of oxygen evolution reaction (OER), water oxidation reaction (WOR), and EDL entropic contributions on catalyst materials such as Pt, RuO_2, IrO_2, NiFe-(oxy)hydroxides and graphene-based single- and dual-atom catalysts.

M.Tech. Dissertation, School of Materials Science and Technology, IIT (BHU) Varanasi — 2018-2019
Advisor, Sanjay Singh, PhD

- Search for potential Weyl semimetal candidates in Heusler alloys using first-principle methods. Mainly used *Quantum Espresso*, *SPR-KKR*, and *python*.

B.Tech. Project, Department of Physics, IIT (BHU) Varanasi — 2016-2017
Advisor, Shradha Mishra, PhD

- Dynamics of a particle moving on Lorentz Lattice Gas on a random 2D collection of points. Ran simulations and analysis using *python*.

INTERNSHIP EXPERIENCE

Summer Research Project, Department of Materials Engineering, Indian Institute of Science — 2017
Advisor, Abhik Choudhary, PhD

- Computed the phase diagrams of binary alloys.
- Implemented the BINGSS source code, which is a Fortran implementation of the CALPHAD method.

Summer Research Project, Mechanical Metallurgy Division, Bhabha Atomic Research Centre — 2016
Advisor, Dinesh Srivastava, PhD

- Investigated the effect of precipitate morphology and distribution on the mechanical behavior of binary Ni-Cr alloy.

Google Summer of Code 2016 — 2016

- Participated with Systers, an Anita Borg Institute Community.
- Used Django, a python-based web framework, to complete the meetup application on the Systers' open-source web portal. Link to the project can be found here.

TEACHING EXPERIENCE

Teaching Assistant, School of Materials Science and Technology, IIT (BHU) Varanasi — 2018-2019
Courses:

- Physical Behavior of Materials
- Introduction to Engineering Materials

HONORS AND SCHOLARSHIPS

Othmer Fellowship for exceptional graduate students 2021
University of Nebraska-Lincoln, Lincoln, NE, USA

IASc-INSA-NASI Summer Research Fellowship Program (SRFP) 2016
India

LEADERSHIP AND VOLUNTEER EXPERIENCE

Conference for Undergraduate Women in Physical Sciences (WoPhys), Volunteer 2021
University of Nebraska-Lincoln, Lincoln, NE, USA

- Organized a lab tour and promoted research in physical sciences to undergraduate female students
- Assisted in organizing the events for undergraduate students

Department Undergraduate Committee (DUGC), Member 2017-2018
School of Materials Science and Technology, IIT (BHU) Varanasi, India

- Contributed to committee meetings as a student representative
- Served as a link between students and department regarding academic affairs

SKILLS AND INTERESTS

- **Software and Packages:** VASP, Quantum Espresso, CP2K, SPR-KKR, VESTA, FullProf Suite, Origin, MATLAB, NumPy, SciPy, Git, LaTeX
- **Languages:** Python, C
- **Operating Systems:** Linux Distros (e.g., Ubuntu, Fedora, Debian, etc.), Windows Systems

PUBLICATIONS

Journals

1. **Payal Chaudhary**, Iman Evazzade, Rodion Belosludov and Vitaly Alexandrov "Computational Discovery of Active and Selective Metal-Nitrogen-Graphene Catalysts for Electrooxidation of Water to H_2O_2" (submitted)
2. **P. Chaudhary**, K.K. Dubey, G.K. Shukla, S. Singh, S. Sadhukhan, S. Kanungo, A.K. Jena, S.C. Lee, S. Bhattacharjee, J. Minár and S.W. D'Souza "Role of chemical disorder in tuning the Weyl points in vanadium doped Co_2TiSn", *Physical Review Materials* 2021, 5(12), p.124201.
3. M. Singh, S. Kumar, M. Alam, V.K. Gangwar, L. Ghosh, D. Pal, R. Singh, P. Shahi, **P. Chaudhary**, K. Shimada and S. Chatterjee "Evidence of surface and bulk magnetic ordering in Fe and Mn doped $Bi_2(SeS)_3$ topological insulator", *Applied Physics Letters* 2021, 118(13), p.132409.

Google Scholar: https://scholar.google.com/citations?&user=C6jAdpMAAAAJ&hl=en