

# CASEY CLARK

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## EDUCATION

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**Doctor of Philosophy in Materials Science and Engineering** anticipated 05/28

University of Utah

GPA: 4.0

**Master of Science in Physical Chemistry** 08/23-12/24

University of Oregon

GPA: 3.46

**Bachelor of Science in Biochemistry** 08/21-12/22

University of Utah

GPA: 3.58

## RESEARCH INTERESTS

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My research focuses on topological quantum materials, specifically amorphous topological insulators, as platforms for next-generation electronics and quantum technologies. I apply ab initio methods alongside AI-driven tools to connect fundamental theory with data-centric materials exploration. My goal is to uncover structure–property relationships for topological materials. I study how composition, strain, and disorder influence quantum and electronic properties in aperiodic systems. These results inform the design and validation of robust, device-relevant materials for demanding environments.

## RESEARCH EXPERIENCE

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**Graduate Research Assistant** 08/25-Present

*Liu & Sparks Groups, Materials Science and Engineering, University of Utah*

- Helped improve the memory utilization & pipeline of KnowMat, an LLM-based tool that takes materials science PDFs & extracts structured data
- Assessed the precision, recall, & F1 score of the LLM-based agentic data extraction tool KnowMat on thermoelectric properties across multiple academic journals
- Currently using VASP, Wannier90, WannierTools, & MLIPs to study bulk amorphous topological insulators

**Graduate Research Assistant** 06/24-12/24

*Hendon Group, Chemistry Department, University of Oregon*

- Obtained the density of states for metal nanoparticles in metal-organic frameworks to assess the tunability of photocatalysis using FHI-aims

- Performed FHI-aims chain calculations to get the activation barrier for the conductivity of protonic defects in 2D metal-organic frameworks
- Computed density functional calculations in VASP to obtain the band structure & density of states for various materials
- Obtained the spin density of diamond NV center spin qubits using VASP

### Undergraduate Research Assistant

10/21-3/23

*Cheatham Group, College of Pharmacy, University of Utah*

- Prepared initial molecular structures & systems using the Chimera software & AMBER software suite
- Ran minimization/equilibration processes for each system using the AMBER software suite
- Ran molecular dynamics simulations for each system using the AMBER software suite & confirmed their progress utilizing the VMD software
- Completed R.M.S.D. and fractional helicity analysis for each system using the AMBER software suite

## PUBLICATIONS

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Sayed HM, **Clark C**, Mohanty T, Sparks T. KnowMat: An Agentic Approach to Transforming Unstructured Material Science Literature into Structured Data. (2025)  
<https://doi.org/10.1007/s40192-026-00455-4>

Diamond, B., **Clark, C.**, Hendon, C. MOF-encapsulation of metal nanoparticles alter the d-band center (2025)  
*In review*

Love, O.D., Lima, M.C.P., **Clark, C.H.**, Cornillie, S., Roalstad, S.M., Cheatham III, T.E. Evaluating the accuracy of the AMBER protein force fields in modeling dihydrofolate reductase structures: Misbalance in the conformational arrangements of the flexible loop domains. *Journal of Biomolecular Structure and Dynamics*. (2022)  
<https://doi.org/10.1080/07391102.2022.2098823>