Atomic Precision as a Path Towards Precious Metal-Free Catalysts

The transition toward a secure energy economy is fundamentally limited by our dependence on critical, scarce metals, driving an urgent need for the development of catalysts composed of earth-abundant elements. Multinary metal chalcogenides offer a rich, tunable design landscape for replacing these precious materials, but their cooperative, multi-center active sites are dififcult to isolate and study directly on extended surfaces. In this talk, I will describe the use of atomically precise molecular clusters as a model platform to resolve these active-site mechanics. By leveraging the structural clarity and rigorous physical and kinetic control possible in these discrete systems, we demonstrate how complex reaction pathways can be deconvoluted to establish clear structure-function relationships, moving the needle from empirical trial-and-error toward rationally guided catalyst discovery. In addition, I will show how well-defined *supra*molecular interactions offer a secondary handle to systematically tune cluster electronic structure and reactivity of these clusters. Overall, these studies highlight how atomic precision can guide the rational design of functional materials tailored for multi-electron energy conversion reactions.

Prof. Gwen Bailey earned her B.Sc. from UBC (Lefevre Medal), Ph.D. from Ottawa as an NSERC CGS-D fellow, and pursued postdoctoral research at Caltech as a Resnick Sustainability Institute and NSERC Postdoctoral Fellow. She joined the University of Minnesota faculty in 2021, where her independent group develops Earth-abundant catalysts for energy conversion. Her accomplishments have been recognized with major national accolades, including the 2023 ACS PRF Doctoral New Investigator Award and the 2026 Beckman Young Investigator Award. Her research has garnered over 50 invitations to lecture at Universities across Canada and the U.S. and at elite national and international meetings such as the Gordon Research Conferences, ACS National Meetings, and 2026 Asian Conference on Bioinorganic Chemistry (Jaipur, India).