INORGANIC SEMINAR

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Atomic Precision as a Path Towards Precious Metal-Free Catalysts

The global transition toward a secure energy economy is constrained by our reliance on scarce, precious metals, highlighting an urgent need for the development of catalysts composed of earth-abundant elements. While multinary metal chalcogenides offer a vast, programmable design landscape for replacing these critical materials, their cooperative, multi-center mechanisms remain a "black box" that hinders rational optimization. In this talk, I will describe the use of atomically precise molecular clusters as a model platform to deconstruct this complexity. Leveraging the unparalleled structural control and rigorous physical and kinetic characterization accessible to these discrete models, we demonstrate how mechanistic complexities can be deconvoluted to yield predictable structure-function relationships, bypassing traditional trial-and-error discovery. In addition, we show how well-defined *supra*molecular interactions provide a secondary handle to rationally tune cluster electronic structure and reactivity. Overall, these studies illustrate how atomic precision enables the rational design of functional materials needed to orchestrate the diverse chemical transformations requisite for a sustainable future.

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