Inorganic Seminar

Monday, May 9, 4 pm

473 Hutchison Hall

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"Atomically Precise Clusters with an Edge: Molecular Insights into Single Atom Catalysts"

Abstract: Understanding and controlling catalytically active sites is the holy grail of nanoscale catalysis, promising to unlock fundamental insights into their mechanism and facilitate the creation of catalysts designed for specific transformations. Atomically precise nanoclusters could enable incorporating molecular precision in the design and mechanistic study of active sites. However, to unlock their potential for catalysis, synthetic innovations are required to prepare monodisperse clusters at scale and to exercise precise control over their surface chemistry and composition. Combining molecular precision and scalability with catalytic competence, our group introduced a family of molecular clusters $M_3Co_6Se_8L_6$ (M = Cr, Fe, Co, Zn, Sn; L = Ph_2PNTol^-) that incorporate three chemically addressable edge sites (M) on the surface of a Co/Se cluster core. This synthetic construct is reminiscent of a broad class of catalytically active edge-doped transition metal dichalcogenide nanomaterials. Hemilabile edge–support interactions stabilize the three edge sites in protected low-coordinate states, positioning them to function as catalytically active sites and enabling the systematic study of electronic metal–support interactions, as well as allosteric effects and multi-site dynamics on the cluster surface. For example, we discovered that $M_3Co_6Se_8L_6$ clusters are not only functional models for heterogeneous single-atom group transfer catalysis, but also a powerful platform to study the dynamics of neighboring active sites in heterogenous catalysts.

Zoom Meeting: https://rochester.zoom.us/j/95869364118

Website: https://events.rochester.edu/event/chemistry_inorganic_seminar_velian

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