

A dissertation defense on

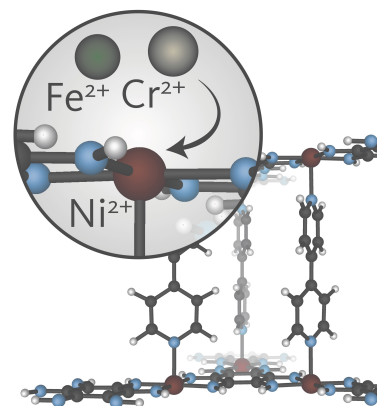
First Principles Studies of The Metal-Organic Interface in Porous Frameworks

ABSTRACT

Due to their generally poor conductivity, metal–organic frameworks (MOFs) have been limited in electrical applications. In this dissertation we explore structural deformation as a route to augmenting the electronic properties of these high surface area materials. We show that, under hydrostatic negative pressure, metallicity can be installed and we also elucidated the covalent characteristic of the metal-organic interface in 2D MOFs.

Continuing our quest, we explore the deformation and phase change within 3D MOFs. Given the stability of metal-organic frameworks under numerous harsh conditions, bonding in MOFs has thought to be static. This project explores the metal-linker interface for a handful of carboxylate-based MOFs under various temperature conditions, which provides evident for dynamic bonding within these frameworks. The metal-linker dynamics resemble the ubiquitous soft modes that trigger important phase transitions offering insights to several important events. We applied the same methods onto Fe-based porous frameworks and elucidated Fe metal centers possess properties such as spin-crossover transition, mixed-valency, and cooperativity which together enhance the material's transport properties.

With these knowledges, we proposed a design principle of retrofitting 2D Fe-based MOFs into 3D analog to achieve highly conductive MOFs. This study contributes a fundamentally new perspective for the design of next-generation conductive metal–organic materials.



When: 4pm (PST), June 14, 2022

Where: 110 Willamette Hall, UO

Remote:

<https://uoregon.zoom.us/my/khoale93>



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