



Department of Chemistry Seminar Series Fall 2022

Friday, September 16, 2022, 3:30 PM - HS1 O112 (Health Sciences)
Host: Fernando Uribe-Romo

Hydrogenic defects in metal-organic frameworks



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Although generally thought of as highly ordered crystals, all metal-organic frameworks contain defects. Some defects may reveal catalytic active sites or hint at competing material phases, while others may result in electronic doping. Modern computational approaches are well-suited to studying the emergent chemistry of these imperfections, and can be used to directly inform experiment and characterization of materials with properties that diverge from those gleaned from crystallography. This talk discusses the chemistry afforded by defects in metal-organic frameworks, with a focus on structural dynamics and adatoms, both promoted by Lewis basic sites within the scaffolds. The utility of these defects will be presented from the perspective of heterogeneous catalyst development.