Nebraska Engineering

FACULTY CANDIDATE SEMINAR

University of Nebraska-Lincoln
Department of Chemical and Biomolecular Engineering

Multi-scale Modeling of Chemical Reactivity in Materials Synthesis

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2:30-4:00 p.m.

Othmer Hall, Room 205

**Refreshments provided*

Abstract

Density functional theory calculations and kinetics can reveal rate-limiting events in complex chemical systems. I will present a case study that shows a detailed formation mechanism of the secondary building unit (SBU) of a chromium terephthalate metal-organic framework (MOF). Metal core and SBU formation control MOF nucleation. A reaction series leading to the formation of an SBU is proposed. The highest barriers involve joining Cr-linker moieties into a di-metal-linker intermediate, and subsequently a three metal-linker core. Terephthalate linkers play a key mechanistic role with carboxylate groups, first joining chromium atoms prior to the formation of bridging oxygens. Subsequent to metal core formation, linker addition reactions occur via multiple pathways due to structural isomers, and are limited by the removal of water molecules in the first chromium coordination shell. A kinetic model based on transition-state theory gave a rate of SBU formation similar to a reported rate of MOF nucleation. The reaction series and kinetic model of SBU formation are the first reported in literature, and build toward developing predictive models of SBU formation, MOF structure assembly, and most importantly the synthesis conditions required. Finally, I will quickly highlight other research projects, fundamental problems and unifying themes, how they fit together, and desired future research directions.

Biography

David is originally from Monterrey, Mexico, where he obtained his BS (2008) in Chemical Engineering with a minor in Industrial Engineering (Ingeniero Quimico Administrador) at the Instituto Tecnologico y de Estudios Superiores de Monterrey. He then went to Iowa State University for his PhD (2013) in Chemical Engineering, under the supervision of Peter J. Reilly, where he did computational research on fatty acid synthesis enzymes as part of the NSF Research Center for Biorenewable Chemicals. Currently he is a Postdoctorate Research Associate at the Pacific Northwest National Laboratory working with Vassiliki-Alexandra Glezakou and Roger Rousseau using computational chemistry and molecular simulation techniques in catalysis and materials synthesis projects.