University of Minnesota
Driven to Discover℠

Department of Chemistry

Seminar

9:45 a.m. Tuesday, March 29, 2016 • 331 Smith Hall

Professor

Coray Colina

Department of Chemistry
University of Florida

Novel nanoporous materials: In silico design

Research interests: understanding and predict ingstructure-property relations in functional materials such as polymeric membranes, biomolecules, and alternative ionic liquids.

Website: https://colina.chem.ufl.edu/

Abstract

Here, we present the results of three exciting opportunities to comprehensively investigate nanoporous materials through the use of molecular simulations. Tailoring and optimization of these materials include: 1) Polymer and organic molecules of intrinsic microporosity (PIMs and OMIMs), which will greatly enhance their suitability as heterogeneous catalysts, adsorbents and gas storage materials. 2) Stilbene containing alternating copolymers, semi-rigid amorphous copolymers, as new polyelectrolytes and other functionalizations for optical applications, and 3) ultra-thin molecular layer-by-layer polyamide membranes which can play a crucial role in the design and understanding of the next generation of reverse osmosis membranes. In all cases, it is anticipated that experimentalists will avoid the peril of performing a large number of difficult synthetic chemistry that would result in no enhancement of microporosity. Concurrent to the above goals, is the generation of large-data sets and the extraction of critical information from that data (e.g., structure factors to understand the intrinsic correlations between structure and properties/behavior) to catalyze materials breakthroughs.

Host: Professor Ilja Siepmann
Refreshments will be served prior to the seminar.