"Atomistic-scale Modeling of Thermal Transport in Nanoporous Materials"

Laura Oliveira, Ph.D.
Assistant Professor
Chemistry Department
University of Wyoming, Laramie, WY

Friday,
October 8, 2021

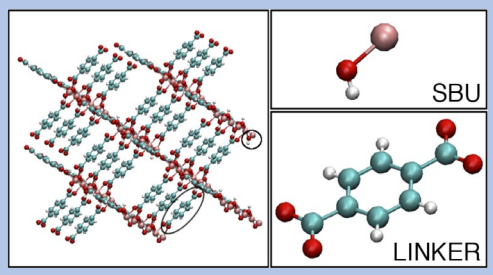
12.10-1.00 PM (MST)

Zoom Link

https://zoom.us/j/93622297036
Meeting ID: 936 2229 7036

Note: Presentation will be projected on Lopez 106 screen, interested faculty members and students are welcome to convene in Lopez 106.

Abstract: The ability to control and manipulate heat goes hand in hand with human progress. This was the case in pre-history when we mastered fire for cooking, heating and defense—and it continues to be true today. As devices get smaller and our ability to nanostructure materials improves, to predict and control heat transport in next-generation materials and devices, it becomes essential to develop an atomistic-level understanding of thermal transport. My research to date has focused on thermal transport at the atomistic scale, including classical molecular dynamics, *ab initio* approaches and heuristic models in a variety of materials. In this talk, I will discuss thermal transport in porous materials, and use that as a segue to briefly discuss a recent project on covalent organic framework membranes for ion separation.



Bio: Laura Oliveira is an Assistant Professor in the Department of Chemistry at the University of Wyoming where she leads the Computational Design of Inorganic Materials Lab, and an NMT alumni. She has undergraduate degrees in Physics and Mathematics from New Mexico Tech. In 2017, Laura graduated with a PhD from the University of California, Riverside. Between 2017 and 2020 she worked as a postdoctoral researcher at the University of Warwick, in the UK, at the Warwick Center for Predictive Modeling. Broadly speaking, her research interests are computer-aided materials design, and using atomistic modeling to understand the physics and chemistry of nano- and bulk-scale phenomena.

NEW MEXICO TECH
SCIENCE • ENGINEERING • RESEARCH UNIVERSITY

Department of Chemistry
Graduate Seminar
Host: Sally Pias