MECHANICAL ENGINEERING
DISSERTATION DEFENSE

The Department of Mechanical Engineering presents:

The Ph.D. Dissertation Defense of

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Engineering Smart Thermal Properties in Metal-Organic-Frameworks

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Dr. Alex P. Greaney, Chairperson

Metal-organic-framework (MOFs) are the most porous materials known to humanity, and thus they attract intensive interest for their huge potential. Hydrogen storage is one of their most important applications. MOFs are promising materials for gas storage and absorption refrigerators--reducing the overall size of the absorption bed. Central to the performance of the MOF is its ability to withdraw heat from the absorbed working gas. The poor thermal conductivity of MOFs limits the refueling time of hydrogen storage because of the removal of latent heat. Currently, to meet DoE's performance targets for hydrogen storage, at least a fivefold increase in thermal conductivity is required. However, their thermal properties have received limited attention. We use molecular dynamics (MD) simulations to study MOFs' thermal transport properties and to identify how they can be exploited to create new materials with smart thermal properties. We “measure” the thermal conductivities of MOFs to test mechanisms for externally tuning the thermal conductivities, and determine if changes in thermal properties of MOFs could be used for chemical recognition. These were performed for the purpose of establishing design principles that can be used in the development of new MOFs with tailored thermal conductivity.

The structure of metal-organic-frameworks (MOFs) is radically different from that of conventional fully-dense crystals and their vibrational behavior differs correspondingly. There are thousands of known MOFs that encompass a wide spectrum of topologies and symmetries. These structures open avenues for engineering materials with entirely new thermal properties. Advancing our theoretical understanding of thermal conduction in these materials, and with it our control over the transport of heat, has a huge potential to impact the way we use and think about heat. More than letting us use heat more efficiently, it will enable us to use heat differently. For example, creating materials in which the thermal conductivity can be externally tuned, and materials that use heat to carry chemical information for chemical recognition.