

# Investigating plasticization and swelling in polymers of intrinsic microporosity (PIM-1) from atomistic molecular simulations

Grit Kupgan<sup>1</sup>, Alexander Demidov<sup>2</sup>, Ping Lin<sup>2</sup> and Coray M. Colina<sup>1,2</sup>

<sup>1</sup>*Department of Materials Science and Engineering, University of Florida, Gainesville, FL*

<sup>2</sup>*Department of Chemistry, University of Florida, Gainesville, FL*

## ABSTRACT

Polymers of intrinsic microporosity (PIMs) are a promising class of polymeric membranes for gas separation. Their design is based on their semi-rigid and contorted backbones, yielding polymers with high free volume architectures. Although PIMs have gained significant attention recently, they can be subjected to undesirable plasticization. Plasticization is defined as the rearrangement of polymers chains due to local swelling of microstructure by condensable penetrants. In this work, we investigated the plasticization behavior in PIM-1 using atomistic molecular simulations. PIM-1 was constructed with Polymatic which is based on a simulated polymerization approach. To account for plasticization and swelling, a hybrid approach is implemented using Monte Carlo (GCMC) and molecular dynamics (NPT). An open-source python package, Pysimm, was used to communicate simulation data between Cassandra and LAMMPS software. When the systems are equilibrated based on proposed convergence criteria, structural and adsorption properties of the simulated samples can be probed at various loading while considering the flexibility of the polymer. This approach allows the study of the effects of plasticization on the performance of PIM-1 for their industrial employment in membrane and pressure swing adsorption applications. Our results showed that the gas loading has a major impact on most structural and adsorption properties. Moreover, we found that plasticization does not always result in the decline of material's performance.