**Title**: Computer Simulation of Hydrogen Storage in *rht* Metal-Organic Frameworks

**Abstract**: Grand Canonical Monte Carlo simulations were performed to investigate hydrogen sorption in two *rht* metal-organic frameworks: PCN-61 and Cu-TPBTM. The simulations were performed using three different hydrogen potentials of increasing realisticness to assess the importance of repulsion/dispersion interactions, charge-quadrupole interactions, and many-body polarization effects. Calculated hydrogen sorption isotherms and isosteric heats of adsorption for both MOFs exhibited undersorption for the models without explicit induction while the polarizable model provides quantitative agreement with experiment. The simulations also produced a variety of other thermodynamic observables that can be directly or indirectly compared to experimental data, such as the isothermal compressibility, radial distribution functions, and dipole distribution. Cu-TPBTM showed a larger hydrogen uptake capacity than PCN-61 due to the presence of the polar amide groups on the linkers. Both of the hydrogen sorption studies performed demonstrated that many-body polarization cannot be neglected when considering high-density hydrogen interacting with highly charged/polar MOFs.