THEORETICAL MODELING OF GAS SORPTION IN MOF'S: THE EFFECTS OF TOPOLOGY AND POLARIZATION. Brian Space , Department of chemistry, University of South Florida, 4202 E. Fowler Ave CHE205, Tampa, FL 33620.

Highly accurate molecular models for gas sorption in MOF's have been developed and applied to both hydrogen and carbon dioxide. Calculated observables such as isosteric heats, sorption isotherms and compressibilities are critically compared with experimental measurements and found to be in excellent agreement. A series of MOF structures have been examined from non-polar to polar and open to confined to assess the what topologies and associated potential energy interactions are responsible for increased sorption. Polarization interactions are shown to be essentially many body in nature and non-negligible considering MOF”s that are promising soprtion candiates.