

EXPERIMENTALLY MOTIVATED PREDICTIVE FORCE FIELDS FOR MODELING MATERIAL SEPARATION, CAPTURE AND CATALYSIS. Christian R. Cioce, Brian Space, Department of Chemistry, University of South Florida, 4202 E. Fowler Ave CHE205, Tampa, FL 33620.

We present modeling of sorption in metal organic framework materials (MOFs) using carefully constructed force fields. The goal is to make quantitative prediction and analysis of experimental observables including sorption isotherms and isosteric heats of sorption. The force fields employed include many body polarization and van der Waals interactions implemented in a computationally tractable fashion. These methods permit predictive accuracy in modeling complex sorption phenomena including sorbate interactions with metals and polar / charged MOFs.