Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Simulation of Photo-isomerization of Functionalized Azobenzene Derivatives PEDRAM TAVAZOHI, ZACHARY HERBERGER, JAMES LEWIS, West Virginia Univ — Photo-isomerization is the process of changing the isomer (*cis*, *trans*) of a molecule using light. In azobenzene this process can be utilized in a Metal Organic Framework (MOF) for adsorption of CO_2. MOFs are created by two major components, metal ions, and organic molecules which are called linkers. The metal ions and linkers can be coordinated in a way that they form a porous material. In the *cis* isomer of azobenzene, the MOFs pore is available to be filled by CO_2, but in the *trans* isomer the pore is filled with a benzene ring. The change from *cis* to *trans* will evacuate the pore if CO_2 is present. The important considerations in using azobenzene photo-isomerization as a photo-switch in MOFs are, the quantum yield of the process, and the wavelength of the light which triggers photo-isomerization. By substitution of the functional groups of azobenzene and using the fewest switches surface-hopping algorithm in FIREBALL to simulate the photo-isomerization process we can tune the properties of the molecule as we desire and predict the best substitution sites for azobenzene functional groups. We studied the effects of functionalizing the molecule with OH, CH_3, NH_2, NO_2 and COOH on isomerization quantum yield.

Pedram Tavazohi
West Virginia Univ

Date submitted: 28 Jan 2016

Electronic form version 1.4