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**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* or *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 usually 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 FSSH 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, $CH_3$, $NH_2$, and COOH on isomerization quantum yield.

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