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Computational study of ZIF with functional groups for CO2 adsorption.

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Greenhouse gases, Carbon Dioxide in particular, has been a main concern for climate change. Zeolitic Imidazolate Framework (ZIF), a sub class of Metal Organic Framework (MOFs), is a 3-dimensional nanoparticle consisting of metal ion (Zn2+) and an organic linker (imidazole) with high chemical and thermal stability. The bond angle between the metal and imidazole has the same 145° angle found in zeolites. These cage like structure are porous and have a high surface area (>1600 m2 g-1). The high surface area is advantageous in several applications such as gas storage, gas separation, chemical sensors etc. ZIFs with its organic imidazole counterpart can be easily modified to add or improve functionality of the materials. Additional functional groups on the imidazole linker such as NO2 groups were found to greatly enhance the CO¬2 adsorption capabilities of ZIFs via a ligand exchange process. In this study a series of functional groups on ZIFs were computed with Grand Conical Monte Carlo (GCMC) simulations by Material Studio to determine whether NO2, SH, F, Cl, Br, CH3, OH, NH2, phenyl and H groups will benefit in improving CO2 adsorption. Our results show that ZIFs with electron withdrawing groups can greatly enhance CO2 adsorption and can easily predict which functional group to synthesis experimentally.

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