Green Synthesis and Testing of ZIF-8 as a Carbon Dioxide Capturing Agent

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Carbon dioxide has been linked to devastating anthropocene changes; rising sea levels, melting glaciers, and increases in natural disasters are all effects of global warming. MOFs are porous structures that can serve as sponges for CO2 as they can be designed to physisorb CO2 molecules by way of direct-air carbon capture. In this investigation, a previously theorized MOF model, ZIF-8, was synthesized using novel green chemistry techniques to determine its utility for carbon capture. The theorized ZIF-8 design was adjusted in Avogadro to screen out misbonded atoms. The lowest level of theory was applied to generate a formula by which to carry out the reaction of linker and node (zinc nitrate-hexahydrate and 2-methylimidazole). When this design failed, a higher level of theory was applied to successfully complete nanoparticle synthesis. The resulting precipitate was activated and exposed to a carbon dioxide-rich environment to imitate point source pollution. When higher levels of computation were applied, a successful synthesis technique for ZIF-8 emerged. To verify that ZIF-8 was synthesized, the PXRD results were compared to those simulated by Vesta. General agreement in trend indicated that the MOF was indeed created. Several rounds of testing showed that the nanoparticles, after exposure to CO2, experienced an average mass increase of 223%, implying that ZIF-8 can capture over three times its weight in carbon dioxide. It is therefore a unique candidate to mitigate global warming.

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