

PROTECTION - SCIENCE AND TECHNOLOGY ADVANCES FOR CHEMICAL AND BIOLOGICAL PROTECTION

Design Of Zeolitic Imidazolate Frameworks Towards A More Efficient Sulfur Dioxide Adsorbent

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Sulfur dioxide (SO₂) is a respiratory tract irritant that aggravates breathing and at high levels, can induce pulmonary edema, pneumonitis, and various other life-threatening conditions. As a byproduct of fossil fuel combustion, SO₂ will remain a toxic industrial chemical (TIC) for the foreseeable future. To prevent exposure in a contaminated environment, filtration devices may be utilized that rely on adsorbents which have a particular affinity for SO₂. Looking to metal-organic frameworks (MOFs) for use as an advanced adsorbent is practical as they often have high surface areas and are easily tuned, allowing for structural modifications, such as expanding pore sizes and ligand functionalization, that may have an impact on their ability to bind efficiently to SO₂. Zeolitic imidazolate frameworks (ZIFs) are of particular interest on account of their ease of synthesis and diverse synthetic availability that host a wide range of features which may allow for optimal SO₂ uptake. Although ZIF-8, which relies on zinc nodes and methyl-imidazole linkers, can be produced in bulk quantities using an aqueous, room temperature synthesis, its topology exhibits a pore-window width of 3.4 angstroms, which is too small to allow for the rapid diffusion of SO₂ throughout the framework. By varying the imidazole linker, either by incorporating functionalized ligands during the initial construction of the material or through post-synthetic ligand exchange (PSLE), pore geometries can be altered and the added functional group's interactions with SO₂ may increase the adsorbent's uptake. ZIFs have been synthesized, exhibiting either a sodalite or gmelinite topology, which has been verified with the use of powder x-ray diffraction (PXRD) and changes in porosity have been monitored with the use of N₂ isotherms. SO₂ adsorption measurements have been taken at 298 K and the variations in uptake help elucidate the impact these modifications have on ZIF's ability to act as a practical SO₂ adsorbent.