Computational Discovery of Highly Sustainable and Efficient Metal-Organic Frameworks for SO2 Capture

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SO2 is a notorious air pollutant, posing significant risks to health and the environment. Traditional flue gas desulfurization methods, such as limestone scrubbing, are characterized by energy inefficiencies and large waste generation – a feeble attempt to ameliorate the detrimental effects of burning fossil fuels. Amidst an urgent need for novel sustainable alternatives, metal-organic frameworks (MOFs) have emerged as promising candidates for SO2 capture due to their unique structure design and vast tunability. However, the time-consuming nature of experimental synthesis and testing greatly limits the search for high-performing MOFs. My work accelerates this critical search by utilizing a computational approach to obtain a comprehensive view of MOF performance and uncover underlying structure-property relationships. Specifically, 3d metal-substituted variants of MOF-74 (M = Sc to Zn) were examined using Density Functional Theory (DFT). By tuning binding affinities via 3d metal substitution, I discovered early transition metal-substituted MOF-74 to be excellent candidates that showed significantly stronger affinity to SO2 and higher SO2/CO2 selectivity. By further analyzing the structural and electronic properties of MOF-74 variants, I found a strong correlation between partial charges of metals and the overall SO2 affinity trend. Occupancy of d-orbitals is hypothesized to be another factor influencing SO2 affinity, where orbital interactions between lone-pair electrons of SO2 and empty d-orbitals of early transition metals led to particularly strong SO2 affinities. These novel insights complement DFT to enable the rapid discovery of high-performing MOFs for SO2 capture, offering key directions for future synthesis and tremendous potential for environmental remediation.

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