Separating Air Using Metal-Organic Frameworks: Influence of the MOF Metal on Oxygen and Nitrogen Binding Energies

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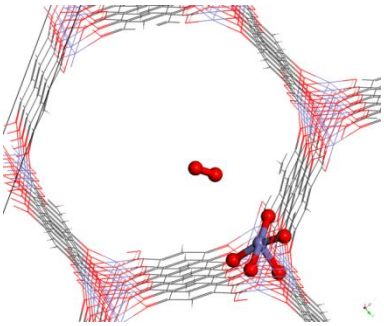
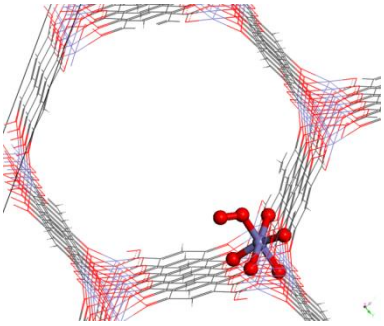
Metal-organic frameworks (MOFs) are a relatively new class of crystalline nanoporous materials that can have very large specific surface areas. By varying the metal and the organic linkers in a MOF, the pore size, net topology, and chemical environment can be finely tuned for specific applications.[1] Recently, MOFs have emerged as a promising class of materials for the effective separation of small molecules.[2-5] MOFs with coordinatively unsaturated metal sites are particularly suited to the separation of oxygen and nitrogen, which is currently achieved by the complex and energy-demanding cryogenic air separation.[4] Several MOFs are known to selectively adsorb oxygen over nitrogen, although none have yet demonstrated selectivities high enough for use in industrial separation.[4]



In order to better understand factors influencing the separation of air by MOFs, metal-substituted variants of two well-known MOFs, MOF-74 and HKUST-1, have been studied using plane-wave-based density functional theory (DFT) calculations. Oxygen and nitrogen binding energies were calculated for 34 MOFs and analyzed as a function of metal. Trends in binding energies as a function of metal will be shown. Binding energies for oxygen and nitrogen are qualitatively consistent with experimental isosteric heats of adsorption.



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References

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