SAND2017-11861PE

Light Gas Separations and Storage with MOFs; Tying the nanoscale science to bulk scale energy and environment applications

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The ability to design, tune and successfully test porous crystalline materials allows for the development and commercialization of materials for many different environmental and energy applications. Metal-organic frameworks (MOFs) have shown great potential in challenging separations of molecules with very similar kinetic diameters. One area of strong focus in our lab is toward a fundamental understanding of the structure-property relationship of selective light gas adsorption in MOFs.

Here we implement a synergistic approach involving predictive molecular modeling, experimental synthesis, and synchrotron crystallographic analysis of known and novel MOF materials. Density functional theory (DFT) calculations were used to measure the binding energy for various gases on coordinatively unsaturated metal sites in MOFs. Various target gases of interest include: O_2, H_2, I_2, Org-I, and hydrocarbons. In one example, emphasis is placed on identifying key structural features for highly selective oxygen adsorption, leading to efficiency improvements through oxy-fuel combustion. A periodic trend in oxygen binding energies was found, with early transition metals exhibiting greater oxygen binding energies compared to late transition metals; this trend was independent of MOF structural type. In another example, highly selective MOFs for I_2 gas are incorporated into novel direct electrical readout sensor devices. Responses are directly related to the structure-property relationship of the MOF to the presence and quantity of adsorbed I_2 molecule. Differential Pair Distribution Function (d-PDF) synchrotron and RAMAN analyses were used to determine guest-host structure relationships on both gas sorbed MOFs and temperature/pressure induced gas retention in MOFs.

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