TODAY'S INNOVATION, TOMORROW'S WARFIGHTER CAPABILITIES

Advances in Fundamental Materials Research

Increased Oxygen Storage Capabilities for the Warfighter Through the Use of Novel Sorbents

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The amount of oxygen that can be carried by the warfighter for various applications is dictated by the amount of gas that can be stored in a canister. An empty canister can be filled with a given amount of gas that is relative to the volume of the canister and the pressure to which it is filled in accordance to the ideal gas law. The amount of gas that can be stored can be increased by the use of high surface area adsorbents such as metal-organic frameworks (MOFs). MOFs are of particular interest for the selective uptake of gases, due to the tailorability of the metal in the inorganic nodes and organic functional groups on the linkers, while maintaining a high surface area and porosity. We have explored a variety of such materials in an effort to understand the sorbent-sorbate interactions at low (less than 1 bar, 15 psi), medium (up to 30 bar, 900 psi), and high pressures (up to 150 bar, 2.25 kspi). We will discuss here the effect of various pendant functional groups on the organic moiety of the MOF, as well as the effect of free metal incorporation through various methods. Density functional theory (DFT) modeling of the binding energy of various organic functionalities with oxygen correlates well to the oxygen uptake by the MOFs studied here.

Varying the chemical composition of the MOF has a large effect on the sorption at lower pressures, while the structural composition (surface area and porosity) has a large effect on the sorption at higher pressures. The application of interest dictates the most beneficial use of MOFs in oxygen storage. For instance, we show at high pressures (140 bar, 2.1 kpsi) MOFs can more than double the storage capacity of a given volume, and we also show the same amount of oxygen that can be stored at 140 bar (2.1 kpsi) can be reduced to a pressure of approximately 30 bar (450 psi) in MOFs. While typical new systems propose canisters that simply can handle higher pressures, we offer a novel approach that allows a reduction in pressure or increase in deliverable oxygen trade space of a given volume, which not only increases effectiveness but also increases the safety of oxygen delivery.

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