Computationally-supported metal organic super container discovery

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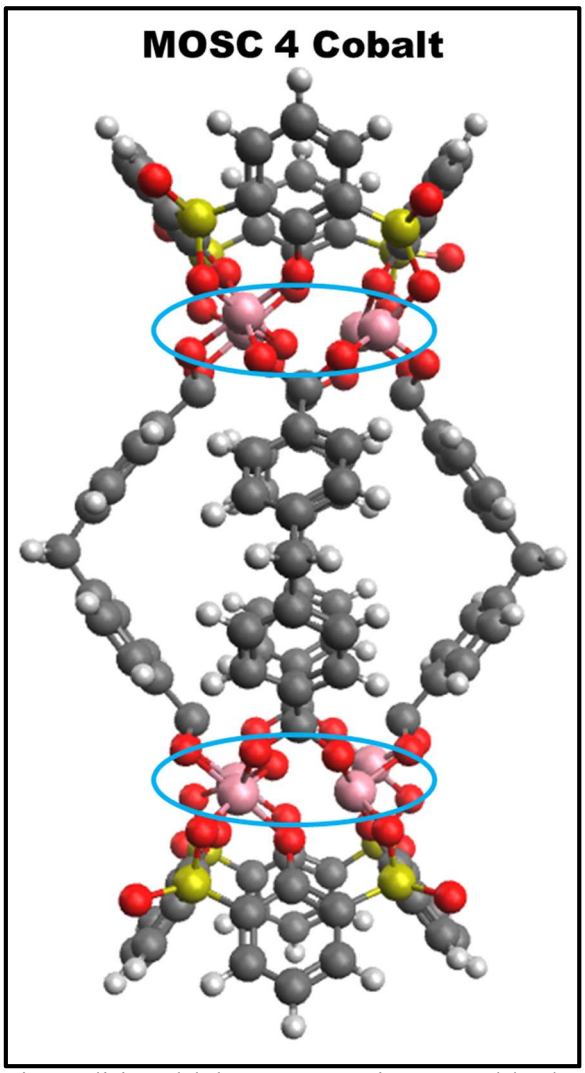

Metal-organic super-containers (MOSCs) have found success in areas such as gas storage, phase separation, and pharmaceutical binding.[1] The MOSC structure can be considered as a single molecular unit of a metal-organic framework (MOF) and is built in much the same way. With dozens of different metals to build into an MOSC, a systematic synthetic analysis in a laboratory setting would be prohibitively expensive with respect to both time and money. A computational survey of different metal-centered MOSCs provides a relatively quick and inexpensive understanding of the different MOSC structures which are possible. The same analysis done with density functional theory (DFT) could be completed in a reasonable time, even with 230 atoms. By utilizing PAW[2] and PBE[3] methods in the Vienna *ab Initio* Simulation package,[4] we can determine the most advantageous MOSC and metal combinations and use it as a guide for experimental work. Various characteristics can be compared among the MOSCs, such as relative energy, band-gap, and theoretical absorption spectra. Comparison of such features can help determine the most stable MOSC structure or most reactive MOSC depending on the desired properties for the particular application. The analysis of the possible MOSC/metal combinations via traditional laboratory settings would take years to complete.

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