Evaluating Metal Organic Frameworks as Smart Nanoporous Preconcentrators for Explosive Sensing

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In order for explosive molecules to be detected, the amount delivered to a sensor must exceed its detection threshold. Pre-concentrators facilitate this process by extracting explosive molecules from the atmosphere and delivering them to sensors in amounts required for reliable detection. With the ability to tailor Metal Organic Frameworks (MOFs), there is hope that a pre-concentrator can be designed to selectively adsorb explosive molecules in the presence of contaminants. In order to test the feasibility of selectively pre-concentrating explosive molecules for detection, molecular simulations of RDX within 5 IRMOFs were performed. The simulations give new insight into the competitive nature of the adsorption and the binding of the explosive molecules to the framework. Adsorption isotherms, mobility of the RDX, the occupancy of each type of cage within the unit cell, and the framework's effect on the configuration of the explosive molecules were investigated by molecular simulation.