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Predicting the Capability of Metal Organic Frameworks to Selectively Pre-Concentrate Energetic Molecules

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In order for explosive molecules to be detected, the amount delivered to a sensor must exceed its threshold. Pre-concentrators facilitate this process by extracting explosive molecules from the atmosphere and delivering them to sensors in amounts required for reliable detection. Current pre-concentrators are not very selective and hence deliver material that is predominately contaminant. With the ability to functionally 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 (1,3,5-trinitroperhydro-1,3,5-triazine) within IRMOF-1 were performed with and without contaminants. The simulations give new insight into the competitive nature of the adsorption and the binding of the RDX to the framework. In addition mobility of the RDX within the framework, the occupancy of each type of cage within the unit cell, and the framework's effect on the configuration of the RDX molecule were investigated by grand canonical Monte Carlo and molecular dynamics.