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Molecular Simulation of Adsorption of Sarin and Simulants on Metal–Organic Frameworks

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Even in 21st century, chemical warfare agents (CWA) remain a threat, and a lot of research and development is aiming to advance protection from CWA. Experiments with CWAs are dangerous and are typically reduced to a minimum. Most of experiments are done on simulants –chemicals which have similar structure, but much lower toxicity. For sarin simulants include dimethyl methylphosphonate (DMMP), diisopropyl methylphosphonate (DIMP), and diisopropyl fluorophosphate (DIFP). Unlike experimental work, molecular simulations are not constrained with the toxicity, so in addition to studies of simulants, simulations can be used for studies of the agents themselves.
In this work we focused on promising adsorbent materials for CWA protection – MOFs - metal-organic frameworks. MOFs are highly porous materials and some of them show strong capacity to capture sarin [1]. We used the selected MOFs from the recent screening study [1] and performed Monte Carlo simulations on adsorption of sarin and its simulants . Although sarin and its simulants have close thermodynamic properties [2], their adsorption behavior can be different, and requires a detailed computational verification. The calculated adsorption isotherms, enthalpy of adsorption and radial distribution functions (RDF) allowed us to select the best MOF for capturing sarin and reveled how similar the interaction between sarin-MOF and simulant-MOF [3]. Based on the calculated properties we have concluded that among all the simulants DMMP demonstrated the closest behavior to sarin. Thereby the results provide insights in selection of the best simulant to study CWA adsorption on MOF's and synthesis new efficient compounds for capturing of chemical warfare agents.
References:

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