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## Applications of MOFs for the chemical warfare agents (CWAs) simulant adsorption

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Chemical warfare agents (CWAs), such as sarin and sulfur mustard, VX chemical components lead to death with only traces of a few micrograms. The use of rapid decontamination of these compounds under harsh conditions remains a great technological challenge. Adsorption is still considered one of the most efficient methods that can be chosen to adsorb such compounds. Metal–Organic Frameworks (MOFs) are efficient materials for the decontamination of CWAs because of their high porosity and tunable reactivity [1]. In this study, a series of stable MOFs, differing in surface area/pore volume, secondary building unit (SBU) connectivity, defects, pore functionalization, and open metal sites were examined in order to assess their adsorption performances. The simulants of CWAs have been taken to mimic the real CWAs [2]. The adsorption microcalorimetry and the force field Monte Carlo simulation are employed to understand the adsorption behaviours of these systems.

Fig. 1. Adsorption microcalorimetry combines adsorption manometry with a Tian–Calvet microcalorimeter, allowing the direct measurement of adsorption energies as a function of amount adsorbed

References:

[1] Hong-Cai Zhou, Jeffrey R. Long, and Omar M. Chem. Rev. 112, 2, 673–674, 2012.

[2] C. Vieira Soares, A.A. Leitão, G. Maurin. Microporous and Mesoporous Materials, 280, 97-104, 2019.

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