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Simulations of physical adsorption of gases in IRMOFs OSARO HARRIOTT, SILVINA GATICA, Howard University — We performed grand canonical Monte Carlo simulations to study the adsorption of noble gases, H_2 and CO_2 in IRMOF-1. The IRMOF is modeled as a simple structure where a cubic lattice is composed of adsorption centers that reproduce the strength of the metallic corners and organic linkers in the real structure. From the adsorption isotherms obtained in our simulations we calculated the isosteric heat of adsorption and compare with available experimental results. Research supported by NSF and ACS, PRF.

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