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Isosteric heat of adsorption of CO_2 in bundles of carbon nanotubes. MAMADOU MBAYE, SIDI MAIGA, SILVINA GATICA, Howard University — Using the grand canonical Monte Carlo method, we have evaluated the adsorption isotherms of CO_2 on the exterior of a bundle of carbon nanotubes. The isosteric heat is a property of the adsorbate that can be calculated from experimental or simulation data, and gives hints of the energy of adsorption and the structure of the adsorbate. From the simulated adsorption isotherms we calculated the isosteric heat of CO_2, Ar and CH_4 and compare with existing experimental data. Research supported by NSF and ACS, PRF.

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