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Isosteric heat of adsorption and uptake of gases in open and closed individual carbon nanotubes MAMADOU MBAYE, SILVINA GATICA, Howard University — We compute by the method of Grand Canonical Monte Carlo the adsorption of argon, methane and hydrogen in the interior and exterior of a single carbon nanotube. The isosteric heat of adsorption is calculated, and the steps observed in the computed adsorption isotherms are interpreted as the formation of cylindrical layers. Our simulations are compared with novel experimental results obtained recently for adsorption in individual carbon nanotubes.

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