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Computer simulations of Ne and CO_2 adsorbed in carbon nanohorns[1] SILVINA GATICA, Howard University, ADAM SCRIVENER, University of Rochester — We compute the equilibrium properties of Ne and CO_2 adsorbed on carbon nanohorns. We modeled the nanohorns as an arrangement of nanometer-size cones composed of carbon atoms. Our method of calculation is the Grand Canonical Monte Carlo technique, where the substrate is considered rigid. We calculate the adsorption isotherms for various temperatures (18K-50K for Ne and 147K - 200K for CO_2). We also calculate the isosteric heat of adsorption and compare with available experimental results.

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