

Gas Adsorption in Novel Environments, Including Effects of Pore Relaxation

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Adsorption experiments have been interpreted frequently with simplified models such as ideally flat surfaces and slit or cylindrical pores. Recent explorations of unusual environments, such as fullerenes and metal-organic-framework materials, have led to a broadened scope of theoretical and simulation investigations. This talk reviews a number of such studies undertaken by our group. Among the topics receiving emphasis are these: universality of gas uptake in pores, novel phases of gases on a single nanotube and the relaxation of a porous absorbent due to gas uptake, all of which studies are motivated by recent experiments.

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