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Commensurate solid phases of Krypton in carbon nanotubes MAMADOU MBAYE, SILVINA GATICA, Department of Physics, Howard University — Recent experiments (Wang et al., 2010) have found evidence of phase transitions of gases adsorbed on a single carbon nanotube. Previous grand canonical Monte Carlo simulations of this system, for the cases of Ar and Kr on zigzag and armchair nanotubes with radius R = 0.7 nm have resembled the experimental results in the case of Ar. However, the prominent, ordered phase found for Kr in both simulations and (classical) energy minimization calculations di_ers from that deduced from the experimental data. A tentative explanation of the apparent discrepancy is that the experiments involve a nanotube of rather large radius (>1.5 nm). We have extended our simulations to nanotubes of larger radius (1-3 nm), zigzag or armchair. In our simulations we found the formation of a layer of the same density than in the experiment, but we believe the layer is not a commensurate solid.

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