Commensurate solid phases of Krypton in carbon nanotubes MA-MADOU 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 differs 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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