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^{4}He Adsorption on a Single Graphene Sheet: Path-integral Monte Carlo Study YONGKYUNG KWON, School of Physics, Konkuk University, DAVID CEPERLEY, Dept. of Physics, U. of Illinois at Urbana-Champaign — We have performed path-integral Monte Carlo calculations to study ^{4}He adsorption on a single graphene sheet, where the ^{4}He-substrate interaction is described by the sum of the helium-carbon pair potentials. Among those proposed to account for helium scattering data on the graphite surface, we employ three different types of the inter-atomic pair potentials; a spherical 6-12 potential, an anisotropic 6-12 potential, and an anisotropic Yukawa-6 potential. Regardless of the choice of the pair potential, a first ^{4}He monolayer is found to show the $C_{1/3}$ commensurate structure at a surface density of 0.0636 Å^{-2} and to go through the domain wall phases for densities above the commensurate one before crystallizing into an incommensurate triangular solid. Below the commensurate density, however, the low-temperature phase of this helium adlayer varies depending on the choice of the ^{4}He-substrate interaction. The calculation based on the spherical pair potentials suggests a superfluid liquid phase at lower densities while incorporation of anisotropy into the helium-carbon pair potential results in a low-density state of a solid with clustered vacancies. Finally we observe van der Waals correlation between the upper monolayer and the one below the graphene sheet. The effects of this interlayer correlation on a possible formation of stable vacancies will be discussed.

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