Path-integral Monte Carlo Study of ^{4}He Adsorption on Carbon Allotropes

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Using a substrate potential described by a pairwise sum of empirical ^{4}He-C interatomic potentials, we have performed path-integral Monte Carlo calculations to study the ^{4}He adsorption on various carbon allotropes. It is found that multiple ^{4}He layers are developed on the carbon surfaces and these helium layers exhibit rich quantum phase diagrams as a result of the interplay between the ^{4}He-^{4}He and the ^{4}He-substrate interactions. On the surface of graphite, specifically, we observe a new stable $C_{7/12}$ commensurate structure in the first ^{4}He layer at the density of 0.111 Å^{-2}, which is not disrupted by the development of the second ^{4}He layer. Furthermore, a second-layer 4/7 commensurate structure relative to the first-layer $C_{7/12}$ solid is found to be at least metastable, opening the possibility of 2D supersolidity [1].

For ^{4}He on α-graphyne, a 2D network of sp-sp^2 hybridized carbon atoms in honeycomb lattice, a Mott insulating state is observed in the first ^{4}He layer at the areal density of 0.0706 Å^{-2} with three ^{4}He atoms occupying each hexagonal cell while the helium atoms form a commensurate triangular solid at a density of 0.0941 Å^{-2} [2]. Here we show that the Ising pseudo-spin symmetry introduced for two degenerate configurations of three ^{4}He atoms in a hexagonal cell can be broken by additional ^{4}He atoms placed at the hexagon vertices and the Mott-insulator to commensurate-solid transition is a transition from a nonmagnetic spin liquid of frustrated antiferromagnets to a spin-aligned ferromagnet under a particle-induced pseudo-magnetic field [2]. Some novel quantum phases manifested by ^{4}He adatoms on other carbon surfaces [3] are also discussed in this talk.

[1] J. Ahn, H. Lee, and Y. Kwon, Phys. Rev. B **93**, 064511 (2016).
[2] Y. Kwon, H. Shin, and H. Lee, Phys. Rev. B **88**, 201403(R) (2013).
[3] J. Ahn, H. Lee, and Y. Kwon, Phys. Rev. B **90**, 075433 (2014).