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^{4}He adsorption on α-graphyne[1] YONGKYUNG KWON, HOONKYUNG LEE, Konkuk University, Seoul, KOREA, DAVID M. CEPERLEY, University of Illinois at Urbana-Champaign, IL61801, U.S.A. — Path-integral Monte Carlo calculations have been performed to study ^{4}He adsorption on a single α-graphyne sheet that is a hexagonal network of *sp*- and sp^2-bonded carbon atoms. Using the ^{4}He-substrate interaction described by a pairwise sum of the helium-carbon inter-atomic potentials, we have found that each hexagon of a graphyne can accomodate one ^{4}He atom at its in-plane center. The first layer of ^{4}He atoms adsorbed on this ^{4}He-attached graphyne sheet with a composite of C_8He_1, exhibits various quantum phases depending on the helium coverage. It is found to be in a Mott insulating state at a coverage of 0.0706 Å^{-2} with three ^{4}He atoms occupying each unit cell while the helium atoms form a commensurate triangular solid at 0.0941 Å^{-2}. With the introduction of Ising pseudospins for two degenerate configurations of three ^{4}He atoms in a hexagonal cell, the transition from the Mott insulator to the triangular solid can be interpreted as a ferromagnetic transition. In addition we find stable formation of zero-point vacancies in the commensurate triangular solid and their roles in possible realization of supersolidity are under investigation

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