

Abstract Submitted
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Commensurate-incommensurate solid transition in the ^4He monolayer on a single γ -graphyne sheet YONGKYUNG KWON, JEONGHWAN AHN, School of Physics, KonKuk University, Korea — We have performed path-integral Monte Carlo calculations to study ^4He adsorption on γ -graphyne. Assuming the ^4He -substrate interaction described by a pairwise sum of empirical helium-carbon interatomic potentials, we find that unlike α -graphyne [1], a single sheet of γ -graphyne is not permeable to ^4He atoms despite its large surface area. One-dimensional density distribution shows layer-by-layer growth of ^4He on γ -graphyne. Partially-filled ^4He monolayers are found to exhibit different commensurate structures depending on the helium coverage; it shows a $\text{C}_{2/2}$ commensurate structure at the areal density of 0.0491 \AA^{-2} , a $\text{C}_{3/2}$ structure at 0.0736 \AA^{-2} , and a $\text{C}_{4/2}$ structure at 0.0982 \AA^{-2} . After going through various domain structures, the ^4He monolayer is completed at the areal density of 0.115 \AA^{-2} where ^4He adatoms form an incommensurate triangular solid. Possible superfluid response of the ^4He monolayer on γ -graphyne is now under investigation.

[1] Y. Kwon, H. Shin, and H. Lee, Phys. Rev. B **88**, 201403(R) (2013).

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