Commensurate-Incommensurate Transition in $^4$He Monolayer Adsorbed on a C$_{60}$ Molecule

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School of Physics, Konkuk University — Path-integral Monte Carlo calculations have been performed to study adsorption of $^4$He on a single C$_{60}$ fullerene molecule. In order to account for helium corrugations on the molecular surface, the sum of all interatomic pair potentials between a carbon atom and a $^4$He atom is used for the $^4$He-C$_{60}$ interaction. The radial density distributions reveal a layer-by-layer growth of $^4$He with the first adlayer being located at a distance of $\sim 6.2 \, \text{Å}$ from the center of a C$_{60}$ molecule. This first layer is found to exhibit various quantum states as the number of adsorbed $^4$He atoms $N$ varies. For $N=32$ the helium layer shows a commensurate solid structure with twenty helium atoms being localized on the tops of the hexagon centers of the C$_{60}$ surface and the other twelve atoms above the pentagon centers. As more $^4$He atoms are added, a commensurate-incommensurate transition is observed. After going through various domain wall states the first layer is crystallized into an incommensurate solid for $N \sim 52$. We find that solid states observed for $N=32, 44$, and $48$ do not show any superfluid response even below 0.2 K while domain-wall fluids formed with $45$ to $47$ $^4$He atoms show significant superfluid fractions below 0.6 K. Finally different quantum states observed in the first $^4$He layer around a C$_{60}$ are compared with phase diagrams determined for the helium monolayer on a graphite surface.

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