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Kinetic Monte-Carlo Simulation of Substrate Vacancy Diffusion in C₆₀ on Ag(111) JOSEPH DULNY III, SANGZI LIANG, JOHN GROH, JORGE SOFO, RENEE DIEHL, The Pennsylvania State University — Recently, clean Ag(111) surfaces with monolayer C₆₀ adsorbates have been studied with scanning tunneling microscopy and low energy electron diffraction. These studies revealed that the C₆₀ forms a commensurate $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$ phase on the Ag(111) substrate and when observed with STM, the C₆₀ molecules appear either “bright” or “dim.” LEED studies showed that these two species of C₆₀ are a result of the C₆₀ taking two different orientations on the Ag substrate, one of which only occurs when the C₆₀ is located over an Ag lattice vacancy. STM also shows the bright and dim C₆₀ molecules change location over time. This “flipping” behavior implies that vacancy diffusion in the Ag lattice is taking place. Here, using the kinetic Monte-Carlo algorithm, we model the diffusion of vacancies in the Ag lattice. Data collected from simulations is compared to experimental data on the flipping rate of the C₆₀ vs. temperature and the bright/dim C₆₀ ratio vs. temperature. Our model tells us that intralayer vacancy diffusion is taking place and that adsorption of C₆₀ on Ag(111) results in vacancy creation in the Ag(111) surface. Additional density functional theory calculations support the conclusions of the model.

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