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C_{60}-Induced Devil's Staircase Transformation on Pb/Si(111) Wetting Layer[1] LIN-LIN WANG, Ames Lab, DUANE D. JOHNSON, Ames Lab and Department of Materials Science and Engineering, Iowa State University, MICHAEL C. TRINGIDES, Ames Lab and Department of Physics, Iowa State University — Density functional theory is used to study structural energetics of Pb vacancy cluster formation on C_{60}/Pb/Si(111) to explain the unusually fast and error-free transformations between the "Devil's Staircase" (DS) phases on the Pb/Si(111) wetting layer at low temperature (˜110 K). The formation energies of vacancy clusters are calculated in C_{60}/Pb/Si(111) as Pb atoms are progressively ejected from the initial dense Pb wetting layer. Vacancy clusters larger than 5 Pb atoms are found to be stable with 7 being the most stable, while vacancy clusters smaller than 5 are highly unstable, which agrees well with the observed ejection rate of ˜5 Pb atoms per C_{60}. The high energy cost (˜0.8 eV) for the small vacancy clusters to form indicates convincingly that the unusually fast transformation observed experimentally between the DS phases, upon C_{60} adsorption at low temperature, cannot be the result of single-atom random walk diffusion but correlated multi-atom processes.

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