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Theoretical Study of Adsorbates-induced Restructuring of Pb flat-top mesas in the Quantum Regime[1] WENGUANG ZHU, University of Tennessee & Oak Ridge National Laboratory, ALEXANDER KHAJETOORIANS, University of Texas at Austin & University of Hamburg, CHIH-KANG SHIH, University of Texas at Austin, ZHENYU ZHANG, Oak Ridge National Laboratory & University of Tennessee — Based on first-principles total energy calculations, we study the adsorption and diffusion of a series of metal adsorbates (Fe, Co and Cs) on flat-top Pb mesas, focusing on their influence on the morphology of the mesas. We found that single Fe and Co atoms can easily dive into the subsurface interstitial sites by overcoming a small energy barrier upon deposition onto the mesa top. In contrast, Cs atoms are able to substitute first-layer Pb atoms via a place exchange process resulting in a surface alloy. This induces a dramatic change on the surface morphology of these mesas as observed in recent experiments. This morphological transformation is characterized by the emergence of Cs-decorated monolayer-high Pb islands which are predominately formed on quantum mechanically unstable regions of the Pb mesas. Connections with experimental observations in other related systems will also be discussed.

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