

Abstract Submitted  
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**QSE induced oscillatory electric field on stepped Pb(111) film and its influence on surface reactivity**<sup>1</sup> XIAOJIE LIU, Beijing Computational Science Research Center, Beijing 100084, China, CAI-ZHUANG WANG, MYRON HUPALO, Ames Laboratory - U.S. Department of Energy, Iowa State University, HAI-QING LIN, Beijing Computational Science Research Center, Beijing 100084, China, KAI-MING HO, MICHAEL TRINGIDES, Ames Laboratory - U.S. Department of Energy, Iowa State University — When the thickness of ultrathin metal films is comparable to the Fermi wavelength, significant effects on the structure stability and the electronic properties emerge due to electron confinement. Using first-principles calculations, we showed that quantum size effects (QSE) can induce oscillatory electrostatic potential and thus alternating electric field on the surface of wedge-shaped Pb(111) films. The alternating electric field has significant influence on adatom diffusion, leading to selective even or odd layer nucleation preference depending on the charge state of the adatom. This QSE induced alternatively modulated electric field is confirmed in growth experiments with the odd-layer preference of Mg adsorption on wedge-shaped Pb/Si(111) films.

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