Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Quantum confinement induced oscillatory electric field on stepped Pb(111) films and its influence on surface reactivity XIAOJIE LIU, Beijing Computational Science Research Center, Beijing, 100084, P.R. China, CAI-ZHUANG WANG, MYRON HUPALO, Ames Laboratory-U.S. Department of Energy, and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, 50011, USA, HAI-QING LIN, Beijing Computational Science Research Center, Beijing, 100084, P.R. China, KAI-MING HO, MICHAEL TRINGIDES, Ames Laboratory-U.S. Department of Energy, and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, 50011, USA — Using first-principles calculations, we showed that such quantum size effects (QSE) can induce oscillatory electrostatic potential and thus alternating electric field on the surface of the wedge-shaped Pb(111) films. The alternating electric field has significant influence on surface reactivity, leading to selective even or odd layer adsorption preference depending on the charge state of the adatoms, consistent with the odd-layer preference of higher Mg coverage on wedge-shaped Pb(111) films, as observed in experiment.

Xiaojie Liu
Beijing Computational Science Research Center,
Beijing, 100084, P.R. China

Date submitted: 13 Nov 2013 Electronic form version 1.4