

Abstract Submitted
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First-principles Study of Pb(111) Nanofilms in the Quantum Regime¹ YONG HAN, RAJ GANESH S. PALA², GUANG-HONG LU³, Department of Material Science and Engineering, University of Utah, Salt Lake City, UT 84112-0610, USA, LI HUANG⁴, Surface Physics Laboratory and Department of Physics, Fudan University, Shanghai 200433, P. R. China, FENG LIU, Department of Material Science and Engineering, University of Utah, Salt Lake City, UT 84112-0610, USA — We report first-principles calculations to investigate surface free energy, interlayer spacing, surface stress, and surface self-diffusion barrier for Pb(111) films in the thickness range of 1 to 31 monolayers, where the quantum size effect (QSE) dominates. We show that similar to surface free energy, all these properties exhibit an oscillation behavior and a beating pattern as a function of film thickness. We will discuss correlations between these properties in terms of QSE.

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