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Quantum Size Effects on Surface Catalysis from First-Principles Studies LI HUANG, School of Physics, Georgia Institute of Technology; Ames Laboratory, XINGAO GONG, Physics Department, Fudan University, ZHENYU ZHANG, Materials Science and Technology Division, Oak Ridge National Laboratory — Using first-principles calculations within density functional theory, we find that the adsorption energies and diffusion barriers of O and CO on quantum (Au+Ag) films show thickness-dependent oscillations. Such oscillations are solely determined by the total thickness of the (Au+Ag) films. The synergetic standing waves formed in the films due to quantum confinement and interference give rise to such quantum oscillation. This result points to potential tunability of the chemical reactivity on ultrathin metal films.

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