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Quantum Size Effects in Nanostructures

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Quantum size effects in metal thin films and metallic clusters are studied using first-principles density functional theory. For metal thin films, Pb(111), Pb(100), Al(110), and Al(111) films up to 30 monolayers are calculated. Significant oscillatory quantum size effects are found on surface energy, work function, and surface relaxations. These oscillations are correlated with the thickness dependence of the energies of confined electrons, which can be properly modelled by an energy-dependent phase shift of the electronic wave function upon reflection at the interface. It is found that a quantitative description of these quantum size effects requires full consideration of the crystal band structure. For metallic clusters, the highly symmetric particles of sizes up to 4 nm (Al_{923} , Pb_{923} , and Au_{309}) in the icosahedral (ico), decahedral, and cuboctahedral (fcc) structures are calculated. We propose a simple scheme to compare their relative stability and to identify the quantum size effect. In addition, the famous Mackay (fcc-to-ico) transition for metallic clusters is investigated by *ab-initio* elastic-band method. The transition path can in general be described by an angular variable \mathbf{s} . The barriers of the Mackay transition for large Al, Pb, and Au clusters are found to be smaller than the thermal energy at room temperature. Finally CO oxidation on metallic clusters will be presented. A catalytic reaction path for CO oxidation on Au_{55} , Ag_{55} , and $\text{Au}_{25}\text{Ag}_{30}$ ico clusters is found with activation energies of less than 0.5 eV. The reaction consists of a peroxolike transition intermediate involving the OOCO configuration. A crucial factor to determine the reaction rate on these clusters is identified as the co-adsorption energy of CO and O_2 on these clusters.