Electronic structure of metal nanoparticles and metallic edges of 2D materials

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Gold nanoparticles and two-dimensional materials are among the most widely-used components of modern advanced materials. We present recent results from Density-Functional Theory (DFT) simulations for the quantum confinement and localization of electrons in such nanostructures. In all cases, we employ the free-software packes GPAW and ASE.

The equilibrium shape of nanoparticles can be calculated from first-principles with the use of the Wulff theorem and surface energies obtained from DFT calculations. The resulting shapes agree very well with microscopy images. Clean Au nanoparticles have truncated octahedral shape, while nanoparticles in CO ga have an almost spherical shape. As a general rule, stronger interactions between the nanoaparticle and its host material result in higher sphericity [1]. Single-electron states are found in these nanoparticles by solving the well-known "particle-in-a-box" problem of quantum mechanics. The boundary condition is that the wavefunction is zero outside the nanoparticle. Apart from the well-known size-dependence of electron excitation energies, we find a strong shape-dependence for these quantum confinement levels. Therefore, the energy spectrum of a nanoparticle could be used as an indirect probe of its shape [2].

A similar analysis leads to new findings for the well-known problem of metallic edges on two-dimensional semiconductors. MoS_2 is found to possess metallic edges. Electrons are localized within 0.5 nm of the zigzag edge, and the energy of these states lies in the middle of the gap of the single-layer [3]. We repeat this calculation for different transition metal dichalcogenides, with different edge terminations and reconstructions, modeled by nanoribbons of variable width. In all cases, we find the same type of edge states that have k-dispersion and are truly metallic. We discuss the Fermi level pinning between the metallic phase at the edge and the semiconducting phase at the interior of the nanostructures.

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