Relativistic effects in quasi-one dimensional systems of metal atoms

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The electronic properties of a system may depend not only on the atomic composition and the geometry but also on the dimensionality. Compared to a three-dimensional bulk, the extension of the system in one or two dimensions may be reduced to below the Fermi wavelength, leading to a quasi-two or quasi-one dimensional system, respectively. Such confinements may lead to transitions between metallic, semiconducting, and insulating states.

Expanding the Dirac equation up to second order in $1/c$, one can distinguish between scalar-relativistic (SR) effects and the spin-orbit coupling (SOC). While the former does not change the symmetry properties of the system compared to a nonrelativistic treatment, the latter does. We present here the results of first-principles, full-potential, density-functional calculations with and without the relativistic first-order corrections up to $1/c^2$ to the Hamiltonian for infinite, periodic, quasi-one dimensional Bi-,Pb-, and Tl-chains. Such chains were recently synthesized inside mordenite channels and on semiconductor surfaces. As expected the relativistic effects are not negligible. The electronic properties of these systems differ from those of the bulk due to the explicit arrangement of the atoms in the chain and/or to the relativistic effects. For example, a linear Pb chain without SOC possesses a metallic behavior, whereas, when including SOC, a band gap opens up because of the splitting of the states and the altered symmetry.

We studied different structures of quasi-one dimensional homoatomic Bi-, Pb-, and Tl-chains. All systems studied here turn out to be extremely soft, i.e. a change in the bond length and/or the angles of the equilibrium geometry requires very little energy, and some are not even stable. On the other hand, the band gap for the semiconducting Pb-chain turns out to be very sensitive against a change in the bond length. Hence, the band gap may be experimentally tuned with only a little external energy or change of the host.