Rational Computational Design of 2D Materials

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Quantum confinement is one of the design principles in nanotechnology. Well-known examples are quantum dots, which are nanocrystals whose electronic band gaps depend crucially on their spatial extension. Thus, it is possible to create light emitting devices with the colour defined by the diameter of the quantum dot. Latest applications include large-scale displays and lasers.

In my presentation I will show that quantum confinement is not restricted to quantum dots and optoelectronic applications. I will show how quantum confinement can be exploited as strategy for the rational design of functional nanomaterials.

The first examples are taken from the field of layered materials, where quantum confinement can be used to tailor the band gap, but also the character of the band gap. For example, transition metal dichalcogenides MX_2 (M=Mo, W, X=S, Se) are indirect band gap semiconductors as bulk and multilayer phases, but direct band gap semiconductors with appreciable photoluminescence signal as single-layer material. These ultrathin materials are also called two-dimensional crystals. The exploitation of quantum confinement gets even more interesting if the symmetry of the material is changed by changing the layer number. For example, by the absence (monolayer) or presence (bilayer) of inversion symmetry in two-dimensional crystals strong spin polarization effects are observed. The strongest quantum confinement effect so far we have predicted for PdS_2, a two dimensional crystal that is semiconducting as monolayer, but metallic as bilayer. Similarly, GeP_3 is a semiconductor in mono- and bilayer form, but metallic for trilayers and thicker stacks.

Another way of exploiting quantum confinement is the application of external fields, most notably electric fields, which are conveniently applied using a gate voltage, and strain fields. I will present various examples where the electronic band gap and/or the density of states are strongly affected by an external gate voltage and by strain fields. For the latter, I will also show some topological phase transitions.

In the final part I will show how quantum confinement can be relieved in molecular crystals, where conjugation can transform local electronic structures to full-featured two-dimensional semiconductors.