Physikalisches Institut

Institut für Festkörpertheorie

CENTER FOR MULTISCALE THEORY AND COMPUTATION

Integriertes Seminar

Aktuelle Probleme dimensionsreduzierter Festkörper

Sondertermin

Ort: Seminarraum 718 (Wilhelm-Klemm-Straße 10)

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Optoelectronic properties of nanostructured devices

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Atomically thin two-dimensional semiconductors have emerged as an interesting class of material systems, both for applications and fundamental studies. For optoelectronic applications like displays, light sources, and photovoltaics, transition-metal-dichalcogenides (TMDs) are an appealing system, as they combine great mechanical strength with high carrier mobility and a direct optical band gap. In this rapidly developing field, attention has recently shifted towards the realization of nanostructures. The generation of localized states, either induced via defects or via systematic confinement engineering, opens the possibility to deterministically generate single-photons or, more generally, provide sources of quantum light. For this purpose, flakes of TMDs have been placed on nanowires, over gold edges and over etched holes to form single-photon emitters. We focus on a different platform, which consists of TMD nanobubbles that develop if air is enclosed during the stacking of layers. The physics governing all of these examples has predominantly been discussed in terms of strain engineering. Due to the high bending rigidity, strain induces large variation of the band gap that can lead to a transition from a direct to an indirect band gap. Another, much less discussed, mechanism is the change of the dielectric environment that also induces strong bandgap variations. We report on results of atomistic tight- binding calculations of different sizes and height-to-diameter ratios of these nanostructures and demonstrate that the formation of confined quantum-dot-like single-particle states is caused by an interplay of strain and dielectric screening. We show that the strain pockets are caused by a crumpling of the material due to its high bending rigidity and discuss the implications of the underlying physics to other TMD-based nanostructures. We also investigate semiconducting TMDs under high excitation and/or high doping conditions. Under such excitation conditions, optical transitions between the first and higher conduction bands are possible, that are analogous to intersubband transitions in conventional quantum well devices. We discuss the carrier density and temperature dependence and show that due to the large Coulomb renormalizations in layered materials, the optical transitions can be tuned into the technologically relevant 1550nm telecom wavelength range. The high absorbances found for single-layer TMDs opens the possibility to utilize TMDCs in novel devices ranging from quantum cascade lasers to novel infra-red photodetectors.

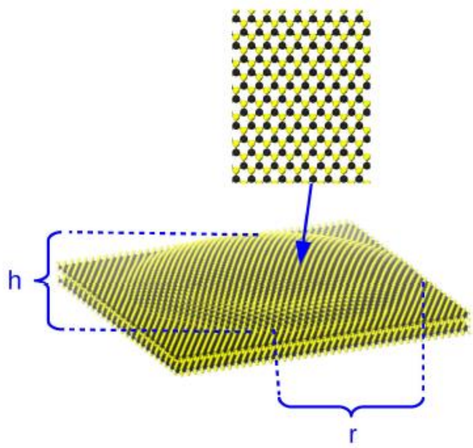

Figure 1: MoS_2 nanobubble

Einladende: Doris Reiter