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S E M I N A R
aus
Halbleiterphysik und Nanotechnologie

Di, 4.4.2017, 13:00 Uhr, Hörsaal für Physik

"Potential and limitations of 2D materials: Insights from computational theory"

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The aim of the presentation is to provide an overview of recent developments in the field of 2D materials beyond graphene. From the materials point of view, the main focus will be on monolayer transition metal dichalcogenides, silicene, and the class of MXenes. A series of examples will be given in order to illustrate how state-of-the-art computational theory based on first-principles materials modeling can contribute to understanding basic physical and chemical phenomena in 2D condensed matter.

Important features of monolayer transition metal dichalcogenides will be introduced, such as the giant spin-orbit coupling and the resulting Rashba spin splitting in polar structures. Limitations of magnetic doping will be discussed. As prototypical example of an interface between two 2D materials, the properties of the semiconductor/metal contact MoS_2/Ti_2CY_2 (Y = F and OH) will be studied. Silicene, the Si analogue of graphene, is of great present interest due to its compatibility with the established Si technology. The material so far cannot be obtained by mechanical exfoliation but can be grown on metallic substrates such as Ag(111). Regrettably, strong interaction with the substrate destroys the Dirac physics. Alternatives will be proposed and the effects on silicene evaluated with respect to technological requirements. While monolayer As is an ordinary semiconductor, it will be demonstrated that fluorination leads to Dirac states, due to structural modifications, and to a topologically nontrivial nature.