Stuttgarter Physikalisches Kolloquium

Max-Planck-Institut für Festkörperforschung
Max-Planck-Institut für Intelligente Systeme
Fachbereich Physik, Universität Stuttgart

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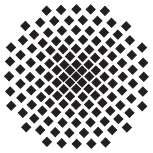

Dienstag, 4. Februar 2020 | **16.15 Uhr** | **Hörsaal 2D5**

Stuttgarter Max-Planck-Institute, Heisenbergstraße 1, 70569 Stuttgart-Büsnau

Electronic structure and properties of a few-layer black phosphorus

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Abstract

I will review some theoretical issues related to a newly discovered two-dimensional material, few-layer black phosphorus (for the case of single layer, also known as phosphorene). This is a direct-gap semiconductor with a gap in Γ point changing from roughly 2 eV in single layer to 0.3 eV in the bulk, with anisotropic and essentially non-parabolic energy spectrum. I will present tight-binding parametrization of electron energy spectrum and its application to large-scale simulations of optical and plasmonic properties. At strong interlayer electric field (or alkali-metal doping) electronic phase transition happens to semimetallic phase with anisotropic Dirac cones. I will discuss consequences of this transition for plasmon spectra and quantum Hall effect. I will also consider single- and two-phonon scattering processes and intrinsic limits on charge carrier mobility in single-layer black phosphorus which turn out to be much more restrictive than for graphene. Electronic structure and properties of transition-metal (Co) and alkali-metal (K) adatoms on black phosphorus will be also considered. As shown both theoretically and experimentally, Co atom demonstrates a high-spin – low-spin transition which can be potentially used for a single-atom memory. Potassium forms nontrivial chain structures reflecting anisotropic electron screening in this material.