



INSTITUT FÜR FESTKÖPERTHEORIE

Sonderseminar

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

Zeit: **Freitag, 07.07.2017, 14:00 Uhr s.t.**

First-principles study of layered BN crystals and BN-Graphene heterostructures

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As a graphene analogue, atomically thin hexagonal BN (h -BN) has recently attracted growing attention because of its wide bandgap and excellent thermal and chemical stability. Indeed, large-area h -BN related quasi-two-dimensional nanomaterials have been fabricated successfully thanks to the progress of modern nanotechnology. According to the reduced charge screening and enhanced electron-electron correlation in these low-dimensional systems, the single and few-layer h -BN nanosheets [1], BN co-doped graphene [2] and BN-graphene heterostructures [3] present novel phenomena that have not been found in bulk h -BN. Such prominent many-body effects, including electron-electron and electron-hole interactions, give rise to unusual electronic structures and significant optical exciton behaviour that pave the way for the promising applications of 2D nanosystems in next-generation optoelectronic and photonic devices. In this talk, we perform first-principles many-body perturbation calculations on quasi-2D BN related nanosystems and BN-graphene heterostructures to explore the origin of these unique electronic and optical properties.

[1] Lijie Ci, *et. al.*, Nature Materials **9**, 430 (2010).

[2] Bo-Yao Wang, *et. al.*, Carbon **107**, 857 (2016).

[3] Zheng Liu, *et. al.*, Nano Lett. **11**, 2032 (2011).

Einladender: Rohlfing