Transport properties of TMDC materials

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1. Introduction

One of the possible material families of the post-Silicon era is the family of the two-dimensional (2D) materials. Whereas graphene was the first member of this group, transition-metal dichalcogenides (TMDCs) provide a large variety of properties. Single-layer molybdenum disulfide (MoS_2), is one of the most intensively studied materials from the TMDC family. Compared to the bulk and few layer MoS_2, the monolayer form is a direct band gap semiconductor that makes it a good candidate for transistor, photodetector, and optoelectronic device applications. Real 2D materials, however, are newer perfect and the structural defects, such as vacancies and grain boundaries can substantially alter the properties of the material.

2. Methods

We investigated the graphene- and MoS_2 structural defects by scanning probe methods and calculated their effect on the transport properties by wave packet dynamics (WPD). Experimentally, the real-space modulation of the LDOS is accessible by Fourier transformation of the topography or tunnelling conductance maps, measured by scanning tunnelling microscopy (STM) [1]. In our WPD formulation [2] the electronic structure of the perfect crystal is described by the kinetic energy operator and the local defects are modelled by the potential energy operator [3], hence the two input quantities of the WPD calculation are the band structure of the perfect 2D crystal which is known from DFT calculations and the localized potential describing the defects.

3. Results

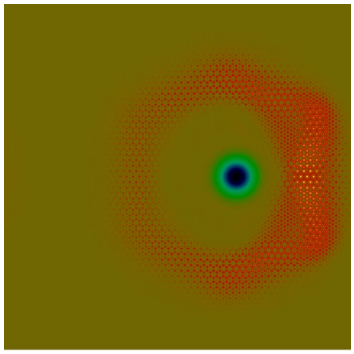

Figure 1 shows the scattering of an electronic wave packet on a localized defect of the graphene surface. This is accomplished by calculating the difference of the time dependent wave functions of a perfect lattice and a lattice containing the localized defect. Though the local potential describing the defect is isotropic, the scattering shows an anisotropic [4] (hexagonal) pattern, because of the anisotropic nature of the graphene dispersion relation. Such anisotropic quasiparticle interferences are clearly seen in scanning probe microscopy experiments [1,3].

Fig. 1. Probability density of the difference wave function, $|\varphi_{with\ pot} - \varphi_{\text{without pot}}|^2$

4. Acknowledgement

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5. References

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