Tunable electronic subband structure and transport in few-layer MoS_2

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Motivated by recent experimental transport measurements on few-layer MoS2 transistors [1,3], we study theoretically the electronic subband structure and transport properties in few-layer MoS_2.

We develop a simple low-energy model for the description of the subband structure of few-layer MoS_2 and apply first-principles DFT calculations to extract values for the involved parameters. We find that the interplay between the (i) weak interlayer coupling, (ii) spin-orbit and spin-valley coupling, and (iii) layer dependent gate potential, results in a highly nontrivial subband structure and wavefunctions whose spatial localization can be tuned with the external gate potential.

Based on a multi-band Boltzmann description of the transport, we demonstrate that this has important consequences for the carrier mobility which, in general, can be expected to be limited by interface disorder. We show that by localizing the subband wavefunctions in the center layer(s) of the sample, scattering off interface disorder can be avoided, thereby significantly improving the transport properties approaching a mobility which is limited by the weaker atomic disorder in the individual layers [2].

Altogether, our findings demonstrate a unique tunability of the electronic structure and carrier mobility in few-layer MoS_2 samples, and shed important light on the origin of experimentally observed resistivity features [1,3] in few-layer MoS2 (see Fig. 1).

References

[1] X. Cui *et al.*, "Multi-terminal transport measurements of MoS_2 using a van der Waals heterostructure device platform", Nature Nano. **10** (2015), 534.
[2] K. Kaasbjerg, T. Low and A.-P. Jauho, "Scattering by atomic vacancies in monolayer MoS_2: Midgap states, symmetry and screening", submitted to Phys. Rev. B (2017).
[3] X. Cui *et al.*, unpublished data.

Figures

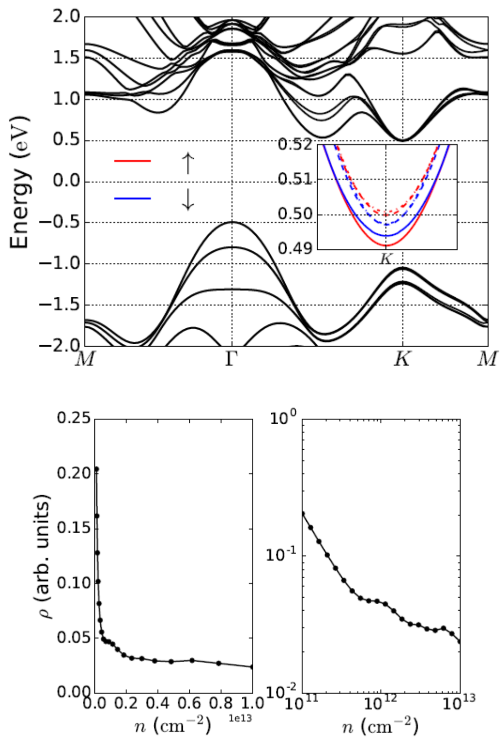

Figure 1: Electronic subband structure (top) and resistivity vs carrier density (bottom) for trilayer MoS_2.. The bumps in the resistivity indicate carrier densities where higher-lying subbands start to become populated, thereby opening additional scattering channels which leads to an increase in the resistivity.