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Unprecedented transport properties of monolayer TMD devices: Experiment and theory

Experimental low-temperature transport in monolayer transition metal dichalcogenides (TMDs; MX_2) is – like in conventional semiconductor heterostructure based 2DEGs – typically found to be limited by Coulomb scattering due to, e.g., charged substrate impurities with mobilities not exceeding μ~5000 $cm^2/(V.s)$ [1]. Here we demonstrate unprecedented transport properties in TMD devices based on *p*-type monolayer WSe_2 showing record-high low-temperature mobilities as high as μ~25.000 $cm^2/(V.s)$ [2]. The mobility surprisingly *decreases* with the carrier density *n*, which is *not* in accordance with charged impurity scattering for which a $\mu \sim n^\alpha$ scaling (with α>0) is anticipated [3].

Using a microscopic, density-functional based method for modeling scattering by realistic atomic-scale defects with the *T*-matrix formalism [4], we investigate the effect of point defects on (i) quasiparticle scattering, (ii) spectral properties, (iii) midgap states, and (iv) transport in 2D TMDs. We demonstrate that the observed density dependence of the mobility is consistent with short-range disorder scattering off atomic point defects, such as, e.g., vacancies, thus pointing to a concomitant breakdown of the widely used Born approximation [4]. At the same time we note that defects in 2D TMDs may act as combined Coulomb and short-range scatterers due to filling of their associated midgap states upon doping [3]. To exclude the existence of the former in our devices, we show that common defects in WSe_2 – in contrast to many other TMDs – do not have filled midgap states above the valence-band edge, and do therefore *not* give rise to Coulomb disorder scattering for *p*-type doping. This points to strongly material, defect and doping (*p* vs *n*) dependent transport properties in monolayer TMD devices.

In conclusion, our combined experimental and theoretical study has shown unprecedented transport properties in monolayer TMD devices with record-high mobilities limited by short-range disorder scattering. This points to extremely clean TMD monolayers with defect densities as low as 10^{11} cm^{-2} as well as high-quality vdW heterostructure devices free of residual charged impurity scatterers.

References

[1] B. W. H. Baugher *et al.*, Nano. Lett. 13, 4212 (2013); H. Schmidt *et al.*, Nano. Lett. 14, 1909 (2014); X. Cui *et al.*, Nature Nano. 10, 534 (2015); X. Cui *et al.*, Nano. Lett. 17, 4781 (2017).
[2] P. Kim *et al.*, unpublished.
[3] K. Kaasbjerg, T. Low, and A.-P. Jauho, Electron and hole transport in monolayer MoS_2: vacancy-induced short-range and Coulomb disorder scattering, to be submitted to PRB.
[4] K. Kaasbjerg, Atomistic *T*-matrix theory of disordered 2D materials: bound states, quasiparticle scattering and transport, in preparation.