# Phonon-limited mobility in single-layer $MoS_2$

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Alongside with the rise of graphene and the exploration of its unique electronic properties, the search for other two-dimensional (2D) materials with promising electronic properties has gained increased interest. Metal dichalcogenides which are layered materials similar to graphite, provide interesting candidates. Their layered structure with weak interlayer van der Waals bonds allows for fabrication of single- to few-layer samples using mechanical peeling/cleavage or chemical exfoliation techniques similar to the fabrication of graphene.[1–4] However, in contrast to graphene they are semiconductors and hence come with a naturally occurring band gap—a property essential for electronic applications.

Single-layer $MoS_2$ is a direct-gap semiconductor with a gap of 1.8 eV.[5] Together with the excellent electrostatic control inherent of two-dimensional materials, the large band gap makes it well-suited for e.g. low power applications. So far, electrical characterizations of single-layer $MoS_2$ have shown $n$-type conductivity with room-temperature mobilities in the range $0.5 - 3$ cm$^2$ V$^{-1}$ s$^{-1}$.[1,2,4] Compared to early studies of the intralayer mobility of bulk $MoS_2$ where mobilities in the range $100 - 260$ cm$^2$ V$^{-1}$ s$^{-1}$ were reported,[6] this is rather low. In a recent experiment the use of a high-$\kappa$ gate dielectric in a top-gated device was shown to boost the carrier mobility to a value of 200 cm$^2$ V$^{-1}$ s$^{-1}$.[4] The observed increase in the mobility was attributed to screening of impurities by the high-$\kappa$ dielectric and/or modifications of $MoS_2$ phonons in the top-gated sample.

In order to shed further light on the measured mobilities and the possible role of phonon quenching from a top-gate dielectric, we have carried out a detailed study of the phonon-limited mobility in single-layer $MoS_2$. The electron-phonon interaction is calculated from first-principles using a density-functional based approach. From the calculated electron-phonon couplings, the acoustic (ADP) and optical deformation potentials (ODP) and the Fröhlich interaction in single-layer $MoS_2$ are inferred. Using these as inputs in the Boltzmann equation, the phonon-limited

mobility is calculated in the high-temperature regime ($T > 100$ K) where phonon scattering often dominate the mobility. Our findings demonstrate that the calculated intrinsic phonon-limited mobility of $\sim 410$ cm$^2$ V$^{-1}$ s$^{-1}$ is dominated by optical deformation potential and polar optical scattering via the Fröhlich interaction. The dominating deformation potentials of $D^0_{\mathrm{HP}} = 4.1 \times 10^8$ eV/cm and $D^0_{\mathrm{LO}} = 2.6 \times 10^8$ eV/cm originate from the couplings to the homopolar and the intervalley polar LO phonon. This is in contrast to experimental observations and theoretical studies for bulk $MoS_2$, where the mobility has been found to be dominated entirely by scattering on the homopolar mode.[6] Furthermore, we show that a quenching of the characteristic homopolar mode which is polarized in the direction normal to the $MoS_2$ layer can be observed as a change in the exponent $\gamma$ of the generic temperature dependence $\mu \sim T^{-\gamma}$ of the mobility. Such a quenching can be expected to occur in top-gated samples where the $MoS_2$ layer is sandwiched between a substrate and a gate oxide.

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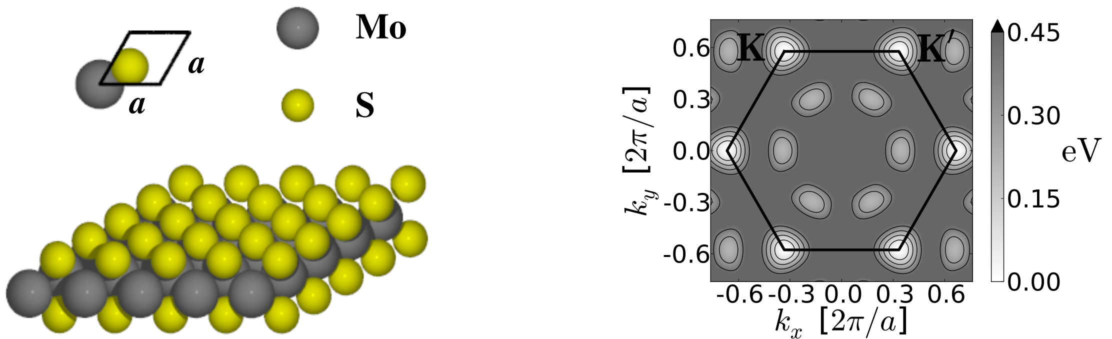


FIG. 1: (Color online) Atomic structure and conduction band of single-layer $MoS_2$. Left: Primitive unit cell and structure of an $MoS_2$ layer with the molybdenum and sulfur atoms positioned in displaced hexagonal layers. Right: Contour plot showing the lowest lying conduction band valleys as obtained with DFT-LDA in the hexagonal Brillouin zone of single-layer $MoS_2$. For $n$-type $MoS_2$, the low-field mobility is determined by the carrier properties in the $K, K'$-valleys which are separated in energy from the satellite valleys inside the Brillouin zone.