Upper Valley and Degeneracy Interplay on the Mobility of Transition Metal Dichalcogenides: Insights from Monte Carlo Simulation

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Outline

Upper Valley and Degeneracy Interplay on the Mobility of Transition Metal Dichalcogenides: Insights from Monte Carlo Simulation

Introduction

- Motivation
- Ensemble Monte Carlo model
- A quick look into degeneracy

Results & discussion

Conclusions

Introduction: **Motivation**

- Transition-metal dichalcogenides in their 2D version are attracting a lot of attention due to their wide and direct bandgap.
- Study of electron and hole transport properties is critical to design devices and to develop future device models.
- Upper valleys and the impact of degeneracy along with screening can bring about interesting transport features worth investigating.
- Monte Carlo model able to capture non-equilibrium transport is an adequate tool to carry out such study.

Introduction:
A quick look into degeneracy

How increasing carrier density inducing degeneracy influences transport?

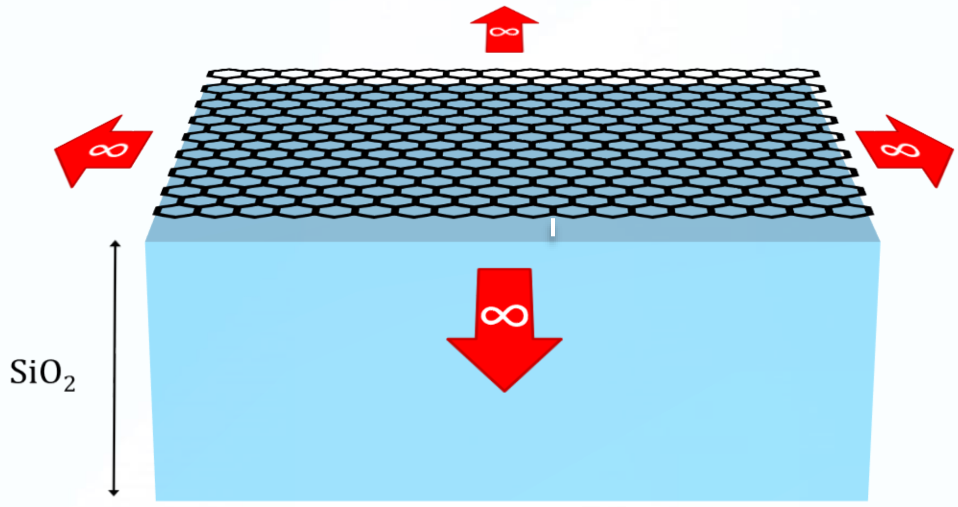
- Fermi level reaches a **higher energy**:
  - **Increased scattering**
  - Easier to reach **secondary valleys** with a larger effective mass (**slower carriers**).

- Many electron/hole transitions due to **phonon emission interactions are forbidden** due to Pauli exclusion principle.
- **Free carriers screen interactions** from polar phonons and impurities.

! **Temperature also becomes a factor in such an interplay**

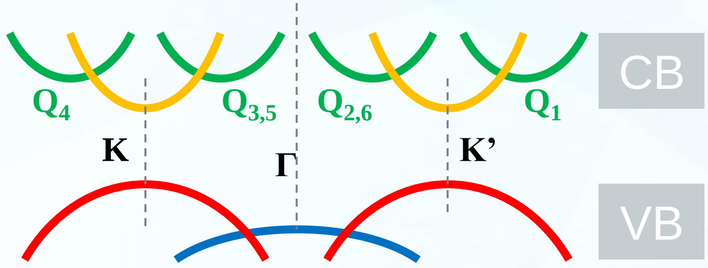
Introduction:
Ensemble Monte Carlo model

- Infinite 2D TMD sheets
- MoS_2, $MoSe_2$, WS_2, WSe_2



- Multi band (e– & h+)
- Multi valley
- ~ 1 000 000 particles
- Scattering mechanisms
  - Intrinsic
  - Substrate
- *n* or *p* (ε_F) and **E** externally fixed

Introduction:
Ensemble Monte Carlo model



Multi-valley effective mass approximation:

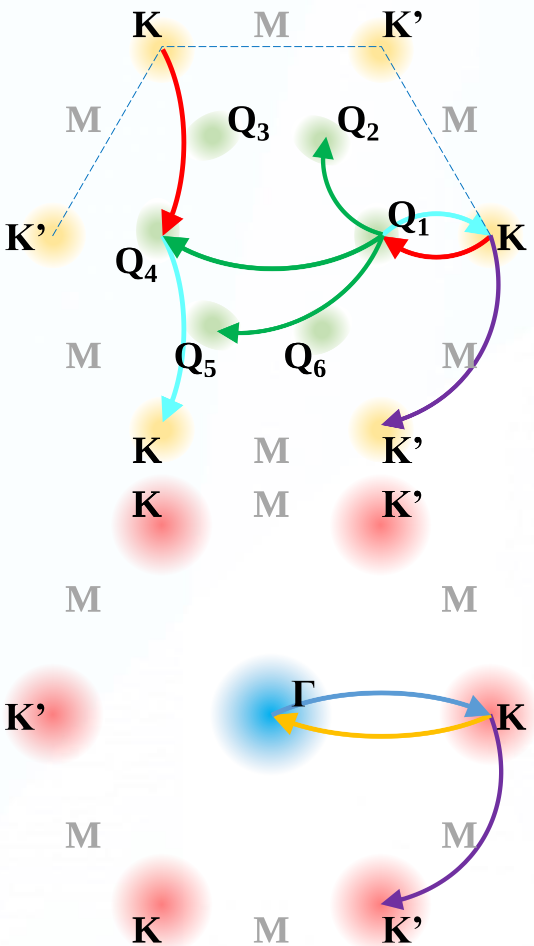
$$\varepsilon(\mathbf{k}) = \frac{\hbar(\mathbf{k}-\mathbf{k_0})^2}{2m^*}$$

- **Conduction band:** 2 primary (K, K') valleys + 6 secondary ($Q_{1\text{-}6}$) valleys
- **Valence band:** 2 primary (K, K' valleys) + 1 secondary (Γ) valley

	Conduction band			Valence band		
	m^*_K (m_0)	$m^{*\,t}_Q/m^{*\,l}_Q$ (m_0)	$\Delta\varepsilon_{Q-K}$ (meV)	m^*_K (m_0)	m^*_Q (m_0)	$\Delta\varepsilon_{\Gamma-K}$ (meV)
MoS_2	0.50	0.62 / 1.00	70	0.58	4.05	148
WS_2	0.31	0.60 / 0.60	67	0.42	4.07	173
$MoSe_2$	0.64	0.80 / 0.80	28	0.71	7.76	374
WSe_2	0.39	0.64 / 0.64	16	0.51	7.77	427

m_0 - electron mass in vacuum

Introduction:
Ensemble Monte Carlo model



- **Carrier scattering with intrinsic phonons**: deformation potential approximation
  - **Intravalley-acoustic** modes

$$\lambda_{D_{1,a}}(\varepsilon) = \frac{m^* {D_{1,a}}^2 k_B T}{\hbar^3 \rho_m {v_a}^2} \int_\theta \frac{d\theta}{\epsilon(q)^2}$$

  - **Intravalley-optical & intervalley** (acoustic + optical)

$$\lambda_{D_{0,a}}(\varepsilon) = g_d \frac{m^* {D_{0,a}}^2}{2\hbar^2 \rho_m \omega_a} \int_\theta \frac{d\theta}{\epsilon(q)^2} \left[n_a + \frac{1}{2} \pm \frac{1}{2} \right] \Theta[\varepsilon \mp \hbar\omega_a(\mathbf{q}) - \varepsilon_0]$$

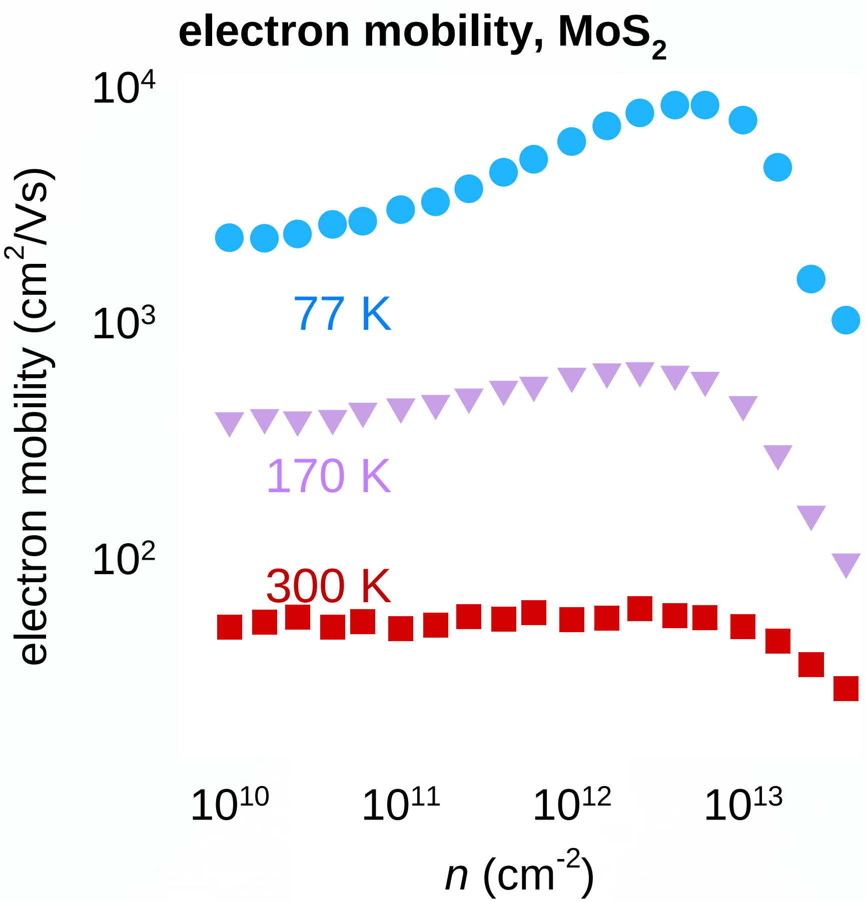
- X. Li et al., *Physical Review B* **87**, 115418 (2013)
- Z. Jin et al., *Physical Review B* **90**, 045422 (2014).

- **Remote substrate polar phonons (SPPs)** through the screened Fröhlich coupling.

- N. Ma and D. Jena, *Physical Review X* **4**, 011043 (2014).
- M. Fischetti et al., *Journal of Applied Physics* **90**, 4587 (2001).

Results & discussion:

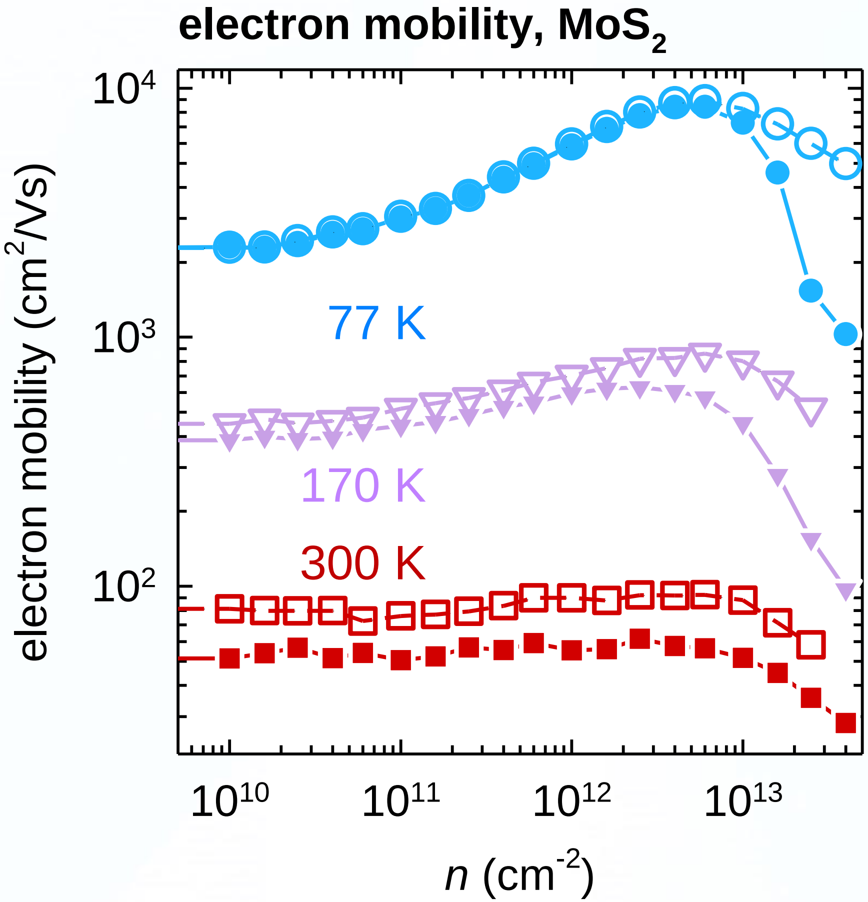
Electron mobility vs. carrier density in MoS_2



Filled symbols: full model
Hollow symbols: screening is excluded

- Low T (77 K & 170 K): Non-linear trend:
  - μ increases in the range $n: 5 \times 10^{10} - \sim 5 \times 10^{12}\ \mathrm{cm}^{-2}$
  - Larger carrier densities lead to a drop below the non-degenerate mobility at $n > 2 \times 10^{13}\ \mathrm{cm}^{-2}$.
- Room T (300 K):
  - μ declines at largest n; no mobility enhancement.

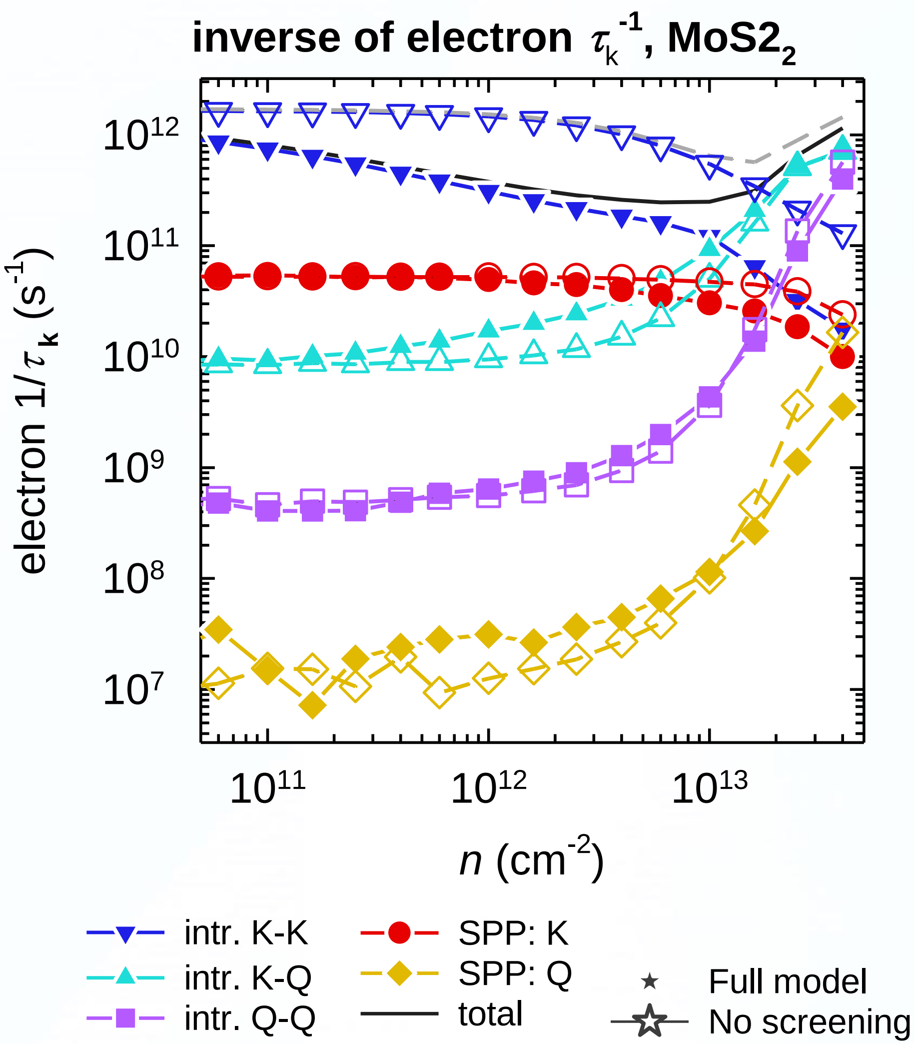
Results & discussion:
Electron mobility vs. carrier density in MoS_2



Filled symbols: full model
Hollow symbols: secondary valleys are excluded

- Simulations excluding the secondary valleys are performed.
- No effect of the Q valley at 77 K until density larger than 10^{13} cm^{-2}.
- Mobility is reduced due to the upper valley occupation for T > 77 K.

Results & discussion:
Electon mobility vs. carrier density in MoS_2



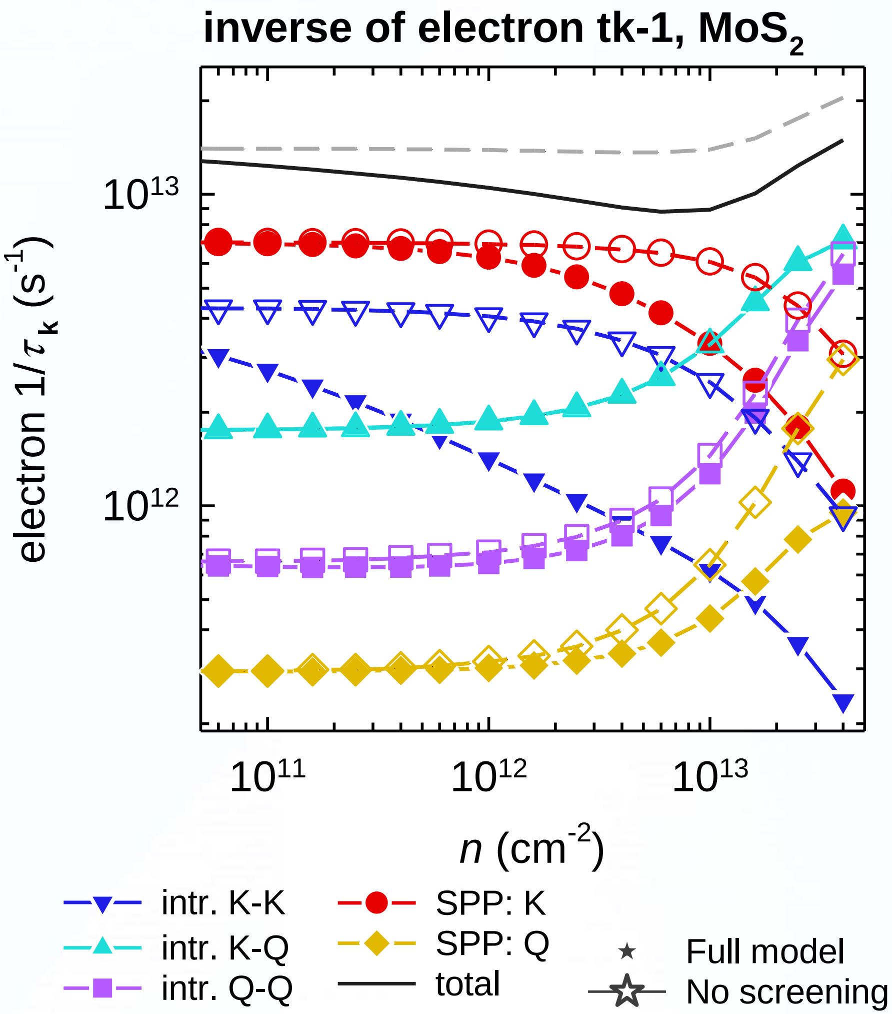
Looking at the inverse of momentum relaxation time…

(T = 77 K)

- The rise in mobility is explained through the decrease of the scattering rate of dominant mechanisms.
- The mobility drop at high concentrations is due to the onset of scattering involving upper valleys, and upper valley occupation itself.

Results & discussion:

Electon mobility vs. carrier density in MoS_2

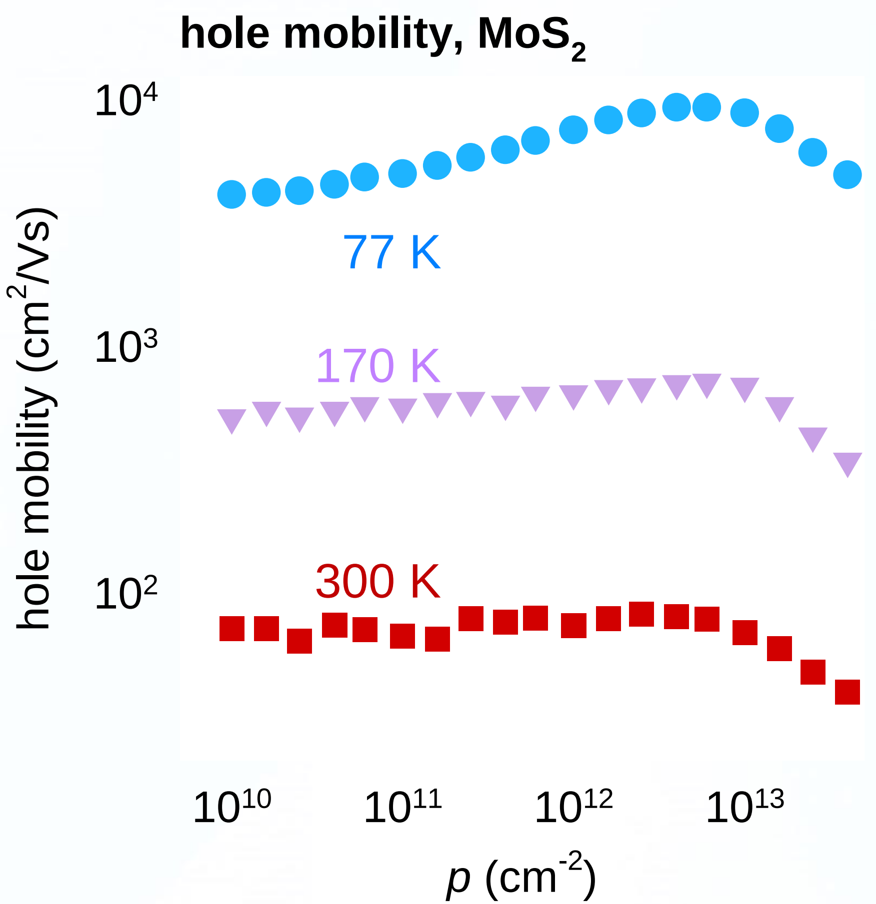


Looking at the inverse of momentum relaxation time…

(T = 300 K)

- SPPs at the K (lower) valleys are dominant as compared to intrinsic phonon interactions.
- Occupation of upper valleys with increasing Fermi level compensates for the drop in scattering interactions in the dominant mechanism.

Results & discussion: **What about holes?**

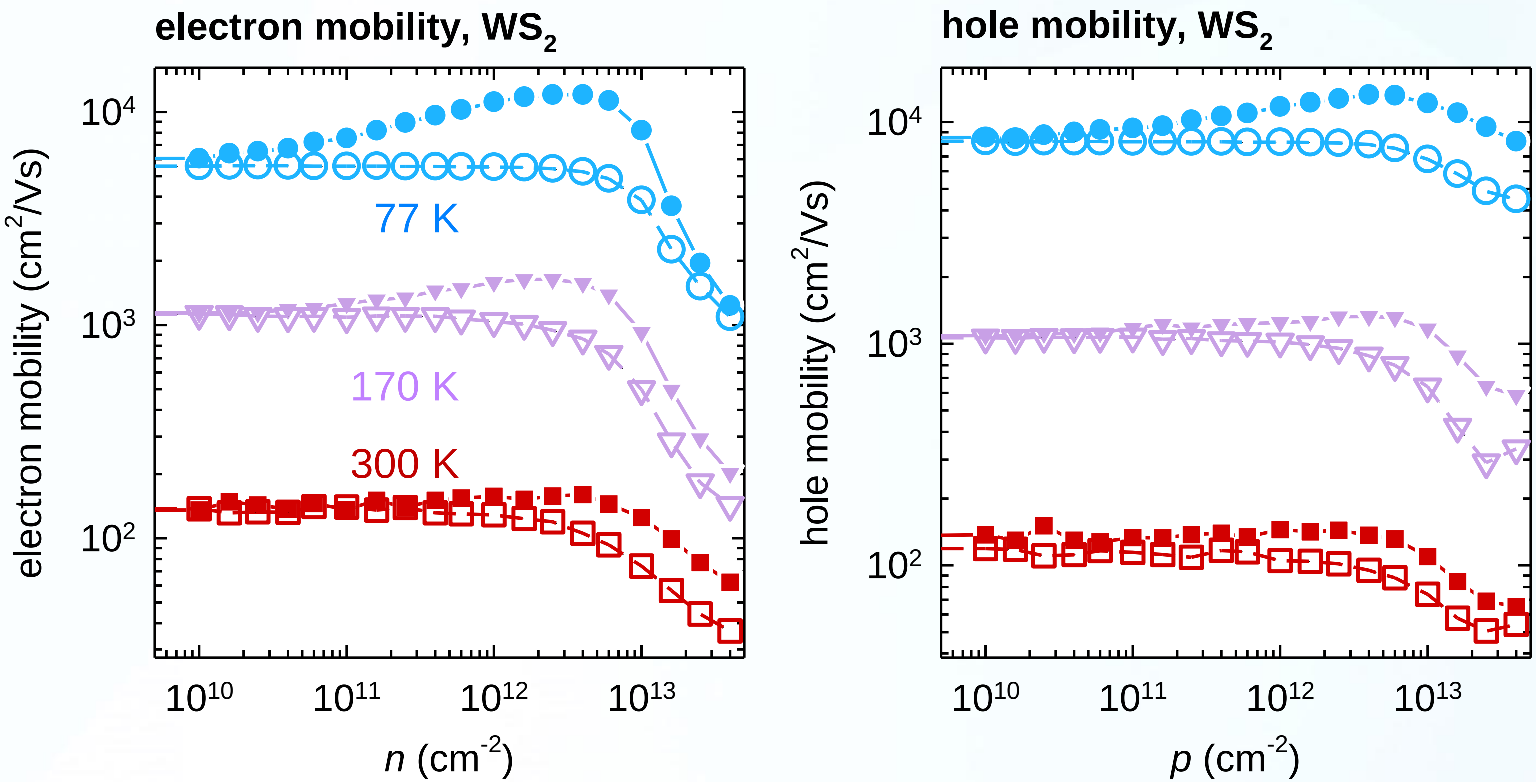


Filled symbols: full model
Hollow symbols: screening is excluded

Similar trend, explainable in alike terms:

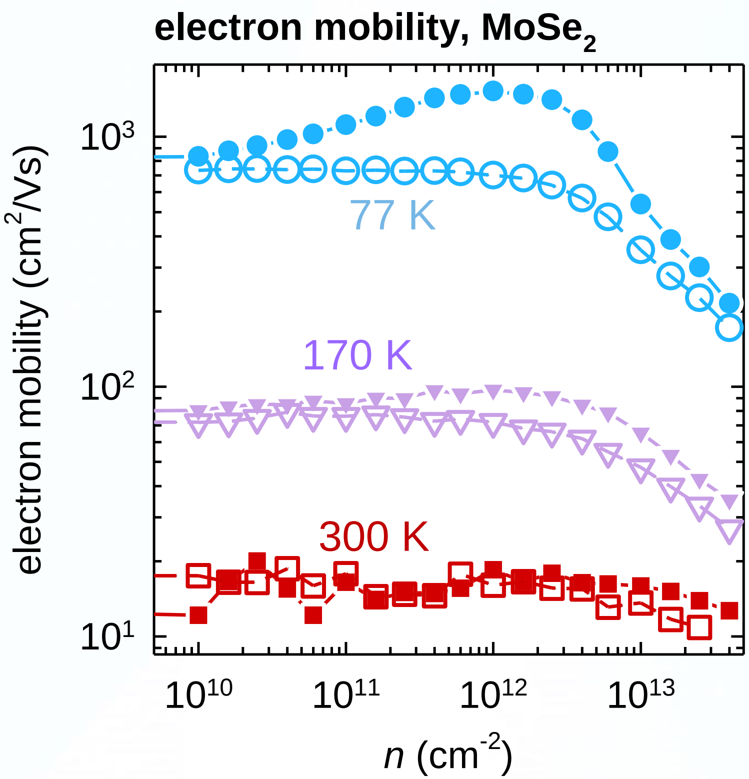
- Hole mobility increase only at a very low T.
- Hole mobility drop above $p \approx 1013$ cm^{-2} is due to holes in the Γ valley + the intervalley scattering.

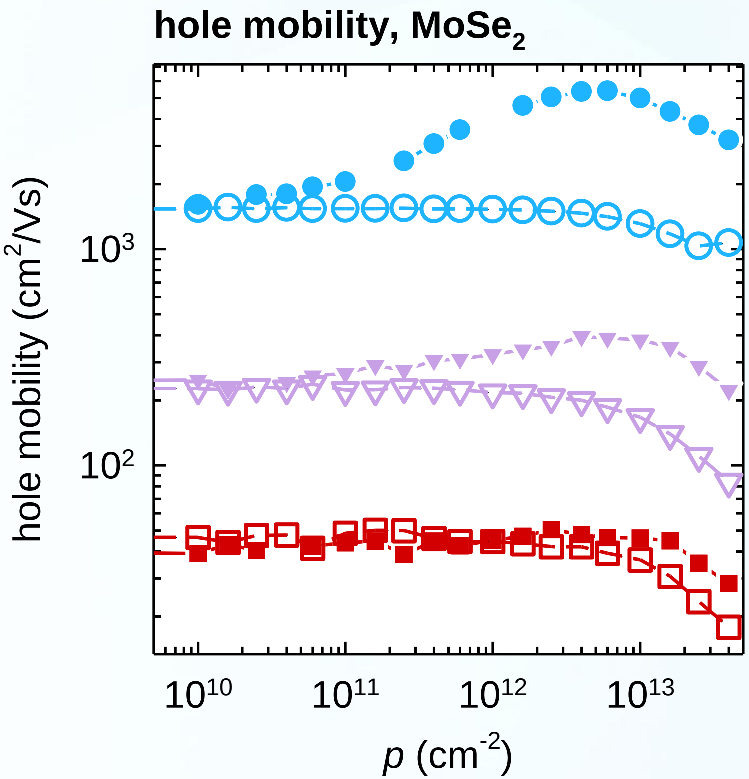
Results & discussion:
TMDs comparison: WS_2



Filled symbols: full model
Hollow symbols: secondary (Q) valleys excluded

Results & discussion:
TMDs comparison: $MoSe_2$





Filled symbols: full model
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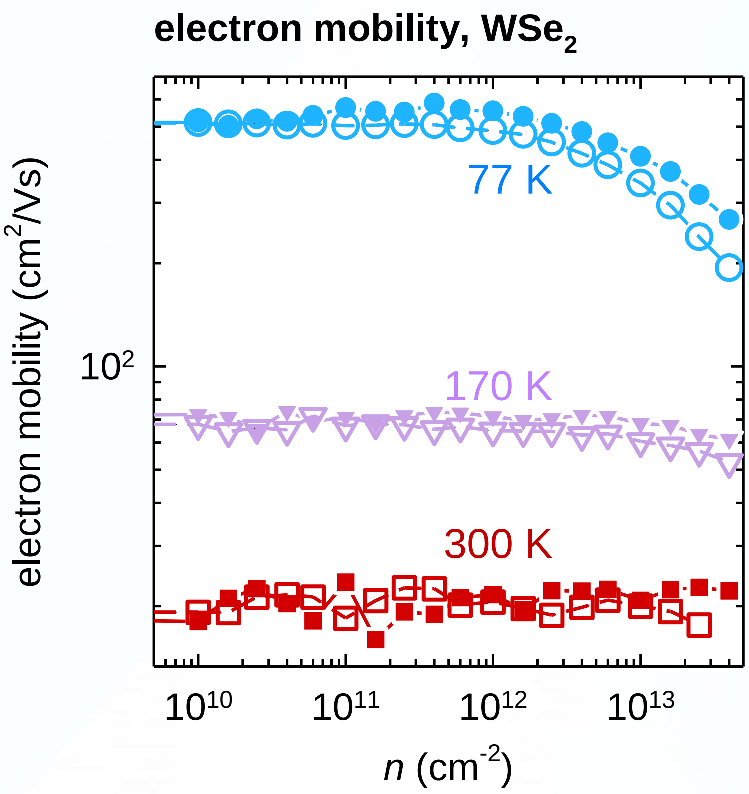
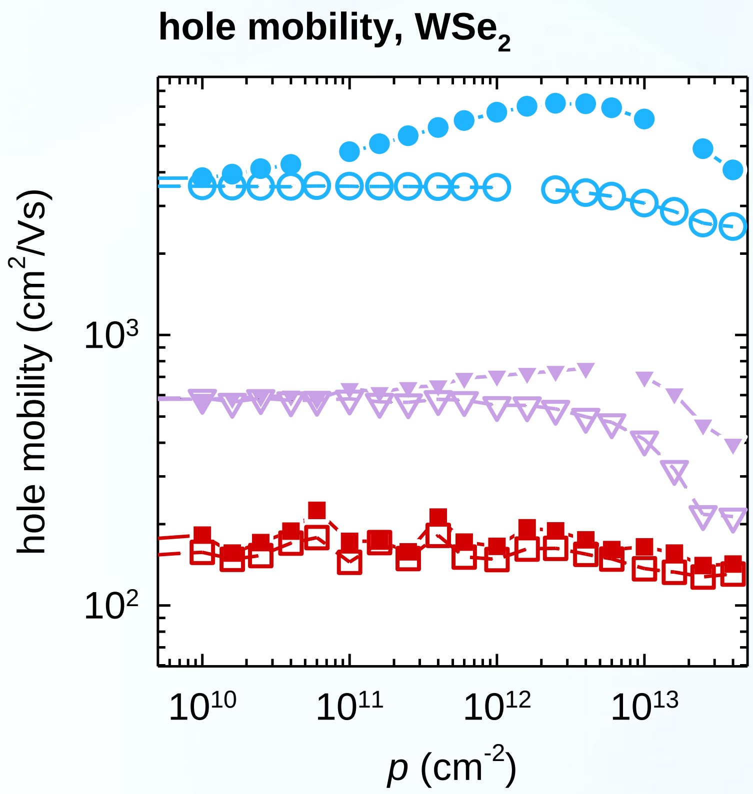
Results & discussion:
TMDs comparison: WSe_2





Filled symbols: full model
Hollow symbols: secondary (Q) valleys excluded

Conclusions

- The complex interactions regarding degeneracy and screening at low field transport in 2D-TMDs have been studied by means of an ensemble MC simulator.
- Predictions of mobility of electrons and holes are larger at low T and intermediate carrier concentrations, when the screening of free carriers and the upper valleys population are considered.
- The reduction of the carrier mobility at high electron/hole densities is mainly due to the occupancy of upper valleys.
- At room temperatures, the upper valley population is large enough to mask the effect of the screening-induced reduction of the scattering in all TMDs studied.
- Most of the observed features can be explained on the basis on relative importance of screened (mostly intra-valley) and unscreened (inter-valley) scattering mechanism, along with a higher valley occupancy.

Related publication

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PAPER

Carrier mobility and high-field velocity in 2D transition metal dichalcogenides: degeneracy and screening

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Supplementary material for this article is available online

Abstract
The effect of degeneracy and the impact of free-carrier screening on a low-field mobility and a high-field drift velocity in MoS_2 and WS_2 are explored using an in-house ensemble Monte Carlo simulator. Electron low field mobility increases to 8400 $cm^2 V^{-1} s^{-1}$ for MoS_2 and to 12 040 $cm^2 V^{-1} s^{-1}$ for WS_2 when temperature decreases to 77 K and carrier concentration is around 5×10^{12} cm^{-2}. In the case of holes, best mobility values were 9320 $cm^2 V^{-1} s^{-1}$ and 13 290 $cm^2 V^{-1} s^{-1}$, reached at similar temperature and carrier concentration conditions while at room temperature these fall to 80 $cm^2 V^{-1} s^{-1}$ and 150 $cm^2 V^{-1} s^{-1}$ for MoS_2 and WS_2, respectively. The carrier screening effect plays a major role at low fields, and low and intermediate temperatures, where a combination of large occupancy of primary valleys and carrier–phonon interactions dominated by relatively low energy exchange processes results in an enhanced screening of intrinsic scattering. For electrons, degeneracy yields to transport in secondary valleys, which plays an important role in the decrease of the low field mobility at high concentrations and/or at room temperature. The high-field drift velocity is not much affected by carrier screening because of an increased carrier scattering with surface optical polar phonons, favouring larger phonon wavevector interactions with small dielectric function values.

Thank you very much for your attention