Intricacies and Limitations of the ab-initio Determination of Electronic Transport Properties in Two-Dimensional Materials

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Two-dimensional (2D) materials have gained wide interest in the field of electronics as a potential channel material in field-effect transistors (FET). The ability of these materials to confine carriers to atomically thin layers provides excellent electrostatics and reduces short channel effects. In addition, their layered nature also reduces/eliminates deviations from ideality, such as surface roughness, dangling bonds, and interface. However, experimental research on these materials is still in the early stages, and most of the predictions are based on theoretical studies. The lack of experimental information, and timely progress made in *ab-initio* ("first principles") methods to calculate band structures, phonon dispersion, and electron-phonon interactions, have made them a popular tool to calculate carrier transport properties of monolayer 2D materials.

Recently we have reported on the electron-phonon scattering rates (see Figs. 1 and 2), mobility (see Table 1) and high-field characteristics of phosphorene [1], silicene and germanene [13,14]. In addition, in Fig. 1 (c), we show our most recent results for the scattering rates in molybdenum disulfide (MoS_2). Throughout our investigations, we have found a large discrepancy among the *ab-initio* predictions of carrier transport properties. Fig. 3 shows the spread of the calculated mobilities found in literature, ranging 20-26,000 $cm^2/(V{\cdot}s)$ for phosphorene [1-6], 130-410 $cm^2/(V{\cdot}s)$ for MoS_2 [7-11], and 0.01-250,000 $cm^2/(V{\cdot}s)$ for silicene and germanene [9,12-16]. Within our precise full-band Monte-Carlo method, we also see discrepancies in the predicted scattering rates (shown in Fig. 1) and mobilities (listed in Table 1) between different well-known *ab-initio* packages.

In this work, we analyze critically the discrepancies we find for the materials listed above. We detail the computational and physical aspects of the various models used in literature. We analyze the underlying causes of the disagreement (ignoring anisotropy, elastic approximation, a coarse discretization) and provide the key ingredients to a precise transport model. With this transport model, we compare different *ab-initio* packages and comment on the reliability of *ab-initio* methods to accurately predict electronic transport properties in novel 2D materials.

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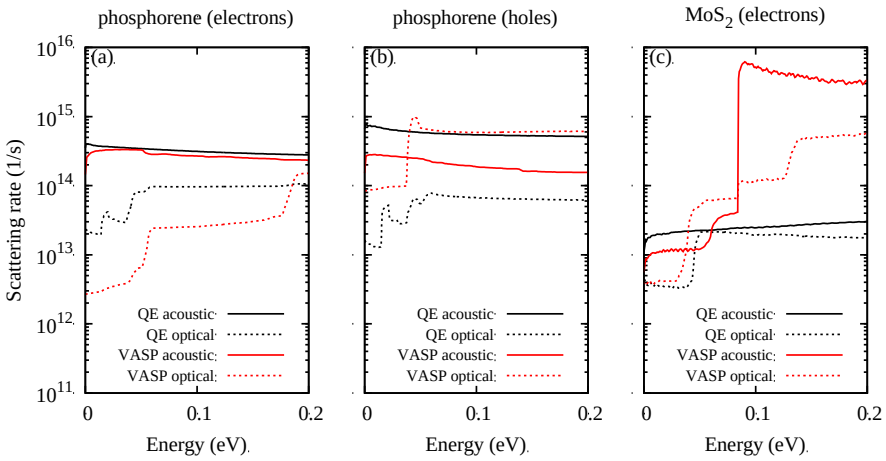

Fig. 1: Carrier-phonon scattering rates at 300K for (a) phosphorene electrons, (b), phosphorene holes, and (c) MoS_2 electrons.

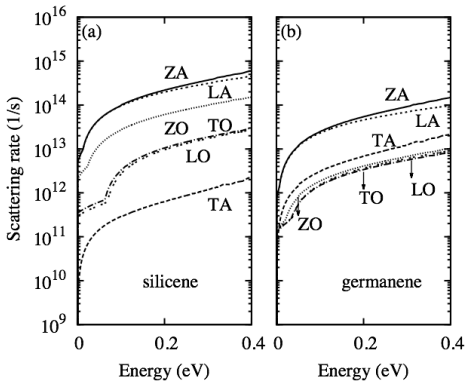

Fig. 2: Electron-phonon scattering rate in (a) silicene, and (b) germanene at 300 K with a 1 nm cutoff for the ZA phonon wavelength.

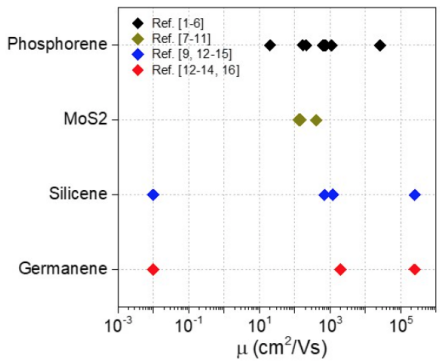

Fig. 3: Spread of the reported mobilities in literature for various 2D materials. Note that the x-axis has a logarithmic scale.

	***Ab-initio* method**	$\mu\left(\frac{cm^2}{V \cdot s}\right)$
Phosphorene	VASP	20
(electrons)	QE	21
Phosphorene	VASP	19
(holes)	QE	19
Silicene	VASP	~10^{-3}
(electrons)	VASP with cutoff*	700
Germanene	VASP	~10^{-3}
(electrons)	VASP with cutoff*	2300
MoS_2	VASP	137
(electrons)	QE	127

Table 1: Low-field carrier mobility μ for various 2D materials, calculated using the full band Monte Carlo method. VASP: Vienna Ab initio Simulation Package, PHONOPY and our own code, uses the finite difference approach. QE: QUANTUM ESPRESSO, uses Density Functional Perturbation Theory. Details are given in Ref. [1]. *: 1 nm cutoff is assumed for the ZA-phonon wavelength in silicene and germanene

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