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Theoretical study of charge transport in mono- and bi-layer phosphorene using full-band Monte Carlo simulations

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Phosphorene, single- or few-layer black phosphorous, has been recently added to the family of two-dimensional (2D) materi- als of interest for nanoelectronics applica- tions. Indeed, phospohorene, like graphene and unlike buckled 2D materials, maintains horizontal (σh) symmetry. Therefore, the cou- pling between electrons/holes and out-of- plane acoustic (ZA) phonons vanishes at first order [1], [2], thus suggesting good phonon- limited charge transport properties. However, reported theoretical estimates of the carrier mobility appear to be excessively optimistic. Indeed, the Bardeen-Shockley deformation potential theorem [3], used to evaluate the electron-phonon coupling, despite its suc- cess when applied to well-known materials, often ignores the anisotropy of the matrix elements and wavefunction overlap-integral. Using such a simplified form of the defor- mation potentials, and also considering only acoustic intravalley processes, mobilities in the range of 700-1100 (300-600) cm^2/Vs have been calculated for electrons (holes) in mono- layers [4], [5]. On the contrary, calculations performed by employing the full matrix elements yield significantly less satisfactory re- sults, $\approx$172 cm^2/Vs for both electrons and holes [6]. Here, by implementing full *ab initio*- based electron/hole-phonon scattering on an extremely fine grid and using the Monte Carlo method, we calculate the phonon-limited mo- bility and high-field characteristics for mono-layer and bilayer phosphorene.

Electron and phonon dispersion. In our study, we obtain the band-structure (Fig. 1) from the density-functional theory (DFT) Vi- enna *Ab initio* Simulation Package (VASP) [7] and phonon spectra (Fig. 2) from the PHONOPY computer program [8]. The relaxed lattice constants obtained are 4.62 A˚ and 3.30 A˚ for mono-layer and 4.52 A˚ and 3.30 A˚ for bi-layer phosphorene. The estimated band gaps are 0.90 eV and 0.50 eV for mono- and bi-layers, respectively. For the bi-layer, the Van der Waals gap obtained is 3.50 A˚ . We find low energy optical modes in bi-layer which are inter-layer modes. Two *k*- space grids, fine and coarse (0.004$A^{\circ -1}$ and 0.013 $A^{\circ -1}$) for the electronic band structure and 0.013 $A^{\circ -1}$ for the phonons) created on the Brillouin Zone, has been used to calculate and tabulate the electronic and phonon dispersions.

Calculation of electron-phonon scattering rates. The scattering rates are calculated numerically using Fermi's Golden rule. The deformation potentials are calculated by full *ab initio* calculations [9] on two grids, fine and coarse, with a size of 0.04 $A^{\circ -1}$ and 0.16 $A^{\circ -1}$ respectively. The density of states is computed using

the 2D version of the Gilat- Raubenheimer algorithm [10]. The scattering rates calculated as a function of carrier kinetic energy, having performed an angular average, are shown in Fig. 3 and Fig. 4.

Charge transport. The Boltzmann transport equation is solved numerically using the full- band ensemble Monte Carlo algorithm to ob- tain the velocity-field and energy-field characteristics. The evaluation of the carrier mobility has been performed by evaluating the diffusion constant D, a procedure that is less affected by stochastic noise [11]. The mobil- ity can then be extracted from D using the Einstein relation.

The velocity-field and energy-field characteristics for transport along the armchair direction for mono- and bi-layer phosphorene are shown in Figs. 5 and 6.

The 300K mobilities for mono-layer and bi-layer are 146 (55) cm^2/Vs and 175 (12) cm^2/Vs for electrons (holes) along the armchair direction and 20 (5) cm^2/Vs and 20 (2) cm^2/Vs for electrons (holes) along the zigzag direction. For monolayers these values are in agreement with Ref. [6] but are much lower than those calculated in Refs. [4] and [5] using isotropic deformation potentials. Note in Figs. 5 and 6 the negative differential mobility resulting from $\Gamma - Q$ intervaley scattering, more noticeable in bilayers because of the smaller energetic separation of these valleys (see Fig.1). Compared to monolayer phosphorene, the higher scattering rate with optical phonons is due to the presence of low-energy inter- layer optical modes. In conclusion, the results obtained do not seem encouraging for the potential use of phosphorene as FETs.

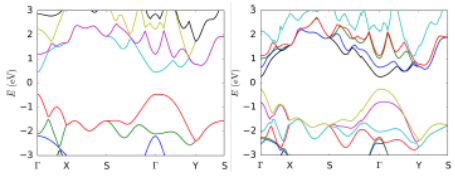

Fig. 1: Electronic band structure of monolayer (left) and bilayer (right) phosphorene obtained using the DFT package VASP[7]

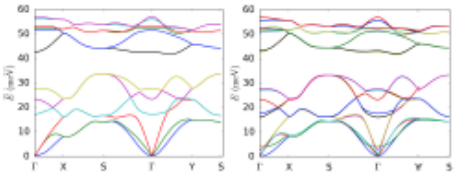

Fig. 2: Phonon dispersion in monolayer (left) and bilayer (right) phosphorene obtained using the PHONOPY program[8]

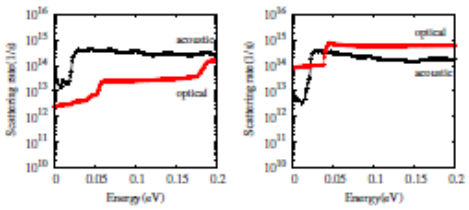

Fig. 3: Electron-phonon (left) and hole-phonon (right) scattering rates at 300 K for monolayer phosphorene.

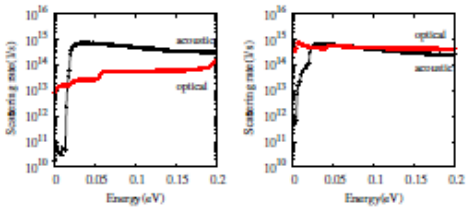

Fig. 4: As in Fig. 3, but for bilayer phosphorene.

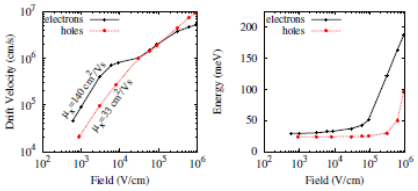

Fig. 5: Drift velocity (left) and average kinetic energy (right) in monolayer phosphorene at 300 K as a function of electric field. Note the negative differential mobility due to strong $\Gamma - Q$ intervalley scattering.

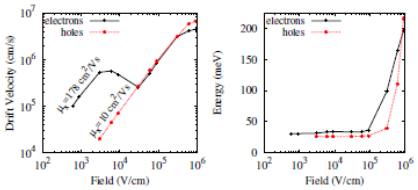

Fig. 6: As in Fig. 5, but for bilayer phosphorene. The negative differential mobility is even more noticeable.

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