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ABSTRACT

In polar compounds, Fröhlich interaction plays an important role in electrical transport, and it is highly dependent on the dimensionality. In two-dimensional (2D) materials, Fröhlich interaction cannot be correctly described by the analytical model available for bulk materials, which prevents the employment of the state-of-the-art first-principles calculation of electrical transport based on maximally localized Wannier functions interpolation. Recently, an approximate 2D Fröhlich model with screened dielectric properties is proposed. Selecting the strong polar material of monolayer InSe, we examine the accuracy of this 2D Fröhlich model by comparing the electron mobility calculated using this model with that based on direct density functional perturbation theory calculations of 2D Fröhlich interaction. It is found that the 2D Fröhlich model can guarantee fairly good results with an advantage of tremendously reduced computational consumption. Using this model, the modulation of the electron mobility of monolayer InSe by the dielectric environment is studied. The electron mobility can be drastically enhanced by coating high-dielectric materials, with room-temperature mobility improved from about 100 $cm^2V^{-1}s^{-1}$ to about 500 $cm^2V^{-1}s^{-1}$, due to the strong suppression of Fröhlich scattering.

I. INTRODUCTION

The reduced dimensionality of two-dimensional (2D) materials unveils some novel physics dramatically different from the three-dimensional (3D) materials and thus provides a new degree of freedom for electronic applications. Numerous 2D materials promising to deliver exciting new electronic technologies have emerged.[1,2] To accelerate the screening of candidates with good electrical transport, the parameter-free computational method enabling accurate prediction of intrinsic carrier mobility is desired. The intrinsic mobility is limited by the phonon, which is the quanta of lattice vibration that perturbs the potential acting on electron. The theory of electron–phonon coupling (EPC) calculation within the density functional theory (DFT) and the density functional perturbation theory (DFPT) has long been established.[3,4] Nonetheless, the implementation has not been made possible until recently since very dense electron and phonon states are required and thus the computational consumption of EPC is a great challenge.

A successful approach to solve the problem of computational feasibility is the maximally localized Wannier functions interpolation of the EPC matrix,[5,6] by which the first-principles calculations are only needed to be conducted on coarse grids. Then, the mobility can be obtained by solving the Boltzmann transport equation (BTE), with scattering limited by EPC interaction.[7,8] This method has been successfully used in non-polar elemental materials.[9–12] In polar compounds, the longitudinal optical (LO) phonons at long wavelength couple strongly with electrons and holes due to long-range Coulomb interaction induced by macroscopic polarization field from the fluctuations of ionic positions, bringing the so-called Fröhlich interaction.[13] Since the stand Wannier functions use localized representations, whereas Fröhlich interaction is not localized in the Wannier basis, the EPC elements cannot be correctly interpolated.[14,15] To address this issue, a polar correction strategy by separating the EPC elements into short-range and long-range contributions is proposed, in which the short-range part is obtained by

Wannier functions interpolation, while the long-range part is directly calculated using an analytical Fröhlich model.[14,15] Considering that the parameters in the analytical model can be calculated from first principles, this method is still in a parameter-free description and keeps high accuracy. This Fröhlich model is strictly derived for the 3D periodic system and behaves superiorly for bulk polar materials.[16–18]

The behavior of Fröhlich interaction is fundamentally affected by the dimensionality. The phonon–momentum dependence of Fröhlich interaction diverges in the long-wavelength limit in the 3D system, whereas it tends to a finite value in the 2D system.[19] The 3D Fröhlich model would overestimate Fröhlich interaction of 2D materials. Current DFT and DFPT calculations generally relied on 3D periodic boundary conditions, which would result in spurious interaction between the 2D systems on its periodic images. Theoretically, the interaction between layers can be weakened by increasing the interlayer distance as long as possible; however, the explosion of computation ensues and thus it is almost impossible to eliminate the long-range interaction completely in practice. By truncating Coulomb interaction in the direction perpendicular to the basal plane with a delicate choice of truncation length,[19–21] the 2D system can be entirely isolated from the start of DFT and DFPT calculations; thus, the EPC matrix automatically including the 2D Fröhlich interaction is obtained[19,21] and has been used to calculate the carrier mobility of 2D polar materials combined with linear interpolation.[22] Nonetheless, relatively large initial grids are needed for linear interpolation, leading to an enormous amount of computational requirement.

Therefore, the polar correction scheme based on Wannier functions interpolation and analytical model calculation is still a priority to boost the pre-research studies. In previous studies of 2D polar materials,[23–25] Fröhlich interaction is either neglected or simply treated with the 3D model. This gives reasonable results for weak polar materials but is no longer in force for strong polar situations. Recently, an analytical model accounting for Fröhlich interaction in 2D materials is established by screening Coulomb interaction.[19] It is urgent to know whether the 2D model can provide satisfactory accuracy especially for materials with a strong polar effect. In this work, by performing first-principles calculations, it is found that the electron mobility of monolayer InSe, calculated without the polar effect, can be an order of magnitude larger than that using the 3D Fröhlich model. Thus, monolayer InSe is well suited for the examination by comparing the electron mobility calculated with the 2D Fröhlich model in the current Wannier functions interpolation framework and that by solving BTE with linear interpolation of the EPC matrix obtained from the direct DFT and DFPT calculations with the truncated Coulomb interaction.

II. METHODOLOGY

The general model incorporating all coupling modes for Fröhlich interaction in the 3D periodic system has been derived as[14,15,26]

$$g^{L}_{mn}(\mathbf{k},\mathbf{q}) = \frac{1}{\sqrt{2\omega_{\mathbf{q}p}}}\frac{i4\pi e^2}{\Omega}\sum_{\mathbf{G}\neq\mathbf{q}}\frac{(\mathbf{q}+\mathbf{G})\mathbf{Z}^{*}\mathbf{e}_{\mathbf{q}p}}{(\mathbf{q}+\mathbf{G})\boldsymbol{\epsilon}(\mathbf{q}+\mathbf{G})} \times \left\langle \psi_{m\mathbf{k}+\mathbf{q}} \middle| e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} \middle| \psi_{n\mathbf{k}} \right\rangle, \quad (1)$$

where $\boldsymbol{\epsilon}$ and $\mathbf{Z}^{*}$ are the dielectric constant and the Born effective charge, respectively, while Ω is the unit cell volume and e is the elemental charge. $\psi_{n\mathbf{k}}$ is the wavefunction of an electron state with band index n and wavevector $\mathbf{k}$. $\omega_{\mathbf{q}p}$ is the frequency and $\mathbf{e}_{\mathbf{q}p}$ is the eigenvector of a phonon labeled by the wavevector $\mathbf{q}$ and mode branch p. $\mathbf{G}$ is the reciprocal lattice vector accounting the periodicity. The summation over $\mathbf{G}$ is performed by the Ewald sum method,[15,26] and the overlap matrix in bra–ket is safely evaluated in the Wannier gauge under smooth phase approximation.[14,15]

Fröhlich interaction is traced back to the long-range Coulomb interaction, which is embedded in Eq. (1) and can be simply expressed as[14,27]

$$W^{3D}(\mathbf{q}) = \frac{4\pi}{\mathbf{q}\cdot\boldsymbol{\epsilon}\cdot\mathbf{q}}. \quad (2)$$

Thus, in order to employ the correction scheme as a 3D system, the Coulomb interaction of the 2D system is needed. As has been discussed in detail,[19,27] it can be approximated with an effective screening as[27]

$$W^{2D}(\mathbf{q}) = \frac{2\pi}{|\mathbf{q}|\left(\varepsilon^{0}_{\text{eff}} + \frac{\mathbf{q}\cdot\mathbf{r}_{\text{eff}}\cdot\mathbf{q}}{|\mathbf{q}|^2}|\mathbf{q}|\right)}, \quad (3)$$

where the screening is characterized by the factor of $\mathbf{r}_{\text{eff}} = \boldsymbol{\epsilon}\cdot t/2$, with t being the thickness of the unit cell, $\varepsilon^{0}_{\text{eff}}$ denotes the average dielectric constant of environment, which is equal to unity for free-standing 2D materials. Equation (1) can be extended to the 2D system by replacing W^{3D} with W^{2D} and replacing Ω with the area of the 2D unit cell.

III. RESULTS AND DISCUSSION

The examination of the 2D Fröhlich model was illustrated in monolayer InSe. It was reported that the hole mobility of monolayer InSe is extremely small,[28] which is two orders of magnitude lower than the electron mobility, due to the much larger effective mass of the hole than that of the electron. Therefore, in this work, we focus on the electron mobility of monolayer InSe in order to make the examination obvious. In addition, since the electron effective mass of monolayer InSe is almost not altered by the spin–orbit coupling and many-body quasi-particle corrections,[28] these effects were not included in the calculations considering the heavy computational task of the direct DFPT calculations of the EPC matrix. The DFT and DFPT calculations were carried out in Quantum ESPRESSO package[29] using norm-conserving pseudopotentials with the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional. The structure was relaxed with $32\times32\times1\mathbf{k}$ meshes and a fixed distance of 20 Å in the direction perpendicular to the basal plane, yielding an optimized lattice constant of 4.05 Å, close to the value of its bulk counterpart.[30] In the cases of Wannier functions interpolation, the electron energy bands, phonon dynamical properties, and the EPC matrix were initially calculated on $12\times12\times1\mathbf{k}$ and $\mathbf{q}$ grids. The related quantities were interpolated to $320\times320\times1\mathbf{k}$ and $\mathbf{q}$ points by EPW package[26] in the calculation of mobility within the framework of iterative solution of BTE.[17,18,31] The convergence of mobility with respect to initial and

final **k** and **q** grids has been ensured (Figs. S1 and S2 in the supplementary material). The predicted mobility without the polar effect is promising, as high as 488 $cm^2 V^{-1} s^{-1}$ at room temperature, as shown in Fig. 1. However, if the polar effect is included with Fröhlich interaction calculated using the 3D model, the obtained mobility decreases dramatically, by 72%–92% in the temperature range of 100–600 K, with a room-temperature value of 69 $cm^2 V^{-1} s^{-1}$. This indicates that polar interaction in monolayer InSe counts for much, and it is hard to confirm what the real mobility should be using the original model of the 3D system.

Therefore, the direct DFPT calculations of all EPC matrix elements for isolated monolayer InSe with truncated Coulomb interaction were performed on $32 \times 32 \times 1$**k** and **q** points. The electron and phonon quantities were still interpolated based on Wannier functions, whereas the EPC matrix was linearly interpolated. The calculated mobility, converged at $320 \times 320 \times 1$**k** and **q** points (Fig. S3 in the supplementary material), is smaller than that of the non-polar case and larger than that using the 3D Fröhlich model as expected, giving a room-temperature value of 144 $cm^2 V^{-1} s^{-1}$, as shown in Fig. 1. Limited by the number of initial grids, the coupling strength of LO phonons around Γ would be underestimated by linear interpolation, and the mobility is probably overestimated. A cunning method can be used for further confirmation,[28] which treats the monolayer as 3D monolayer/vaccum superlattices, and the 3D Fröhlich model is employed. The initial **k** and **q** grids are $12 \times 12 \times 2$, and they are interpolated to $320 \times 320 \times 6$ to achieve convergence (Fig. S4 in the supplementary material).

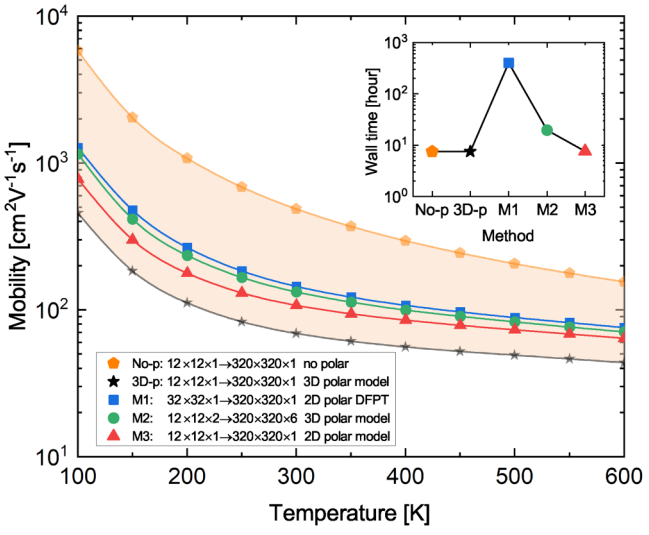

FIG. 1. Electron mobilities of monolayer InSe calculated by different treatments of polar interaction. No-p: without polar interaction; 3D-p: including polar interaction using a 3D Fröhlich model; M1: direct DFPT calculation of the EPC matrix with truncated Coulomb interaction combined with linear interpolation; M2: treating the monolayer as a 3D monolayer/vacuum superlattice and meshing in the out-of-plane direction for the employment of the 3D Fröhlich model; M3: using the 2D Fröhlich model. The inset shows the computing times corresponding to each method under the same computational resources.

The calculated mobilities are close to the results of direct DFPT calculations, with a room-temperature value of 132 $cm^2 V^{-1} s^{-1}$, which to some extent implies that the initial grids in direct DFPT calculations are relatively sufficient. Therefore, it is justified to conclude that the electron mobility of monolayer InSe should be in the order of 100 $cm^2 V^{-1} s^{-1}$ at room temperature.

To compare with Ref. 28, by treating monolayer as 3D monolayer/vacuum superlattices, the mobilities are also calculated under the self-energy relaxation time approximation (SERTA) of BTE. The obtained mobility is only about 83 $cm^2 V^{-1} s^{-1}$ at room temperature, smaller than the value of 120 $cm^2 V^{-1} s^{-1}$ predicted in Ref. 28. We noticed that the local density approximation (LDA) pseudopotentials were used in Ref. 28, thus the mobilities using LDA are calculated and larger values than that of PBE are obtained (Fig. S5 in the supplementary material). The mobilities calculated under SERTA using LDA agree well with Ref. 28, giving a room-temperature value of 118 $cm^2 V^{-1} s^{-1}$. The impact of different pseudopotentials on mobility has been revealed in previous studies,[11,32] mainly due to the difference of band structures. In spite of the discrepancy resulted from PBE and LDA, the comparison of different treatments of polar interaction in this work is still reasonable since all calculations are carried out with the same PBE pseudopotentials. It is also found that the solution under SERTA is obviously different from the iterative solution of BTE especially at high temperatures in all calculations (Figs. S5 and S6 in the supplementary material), indicating the significance of the iterative solution, which is usually important in strong polar materials.[17,18]

By adopting a 2D Fröhlich model, the calculated mobilities are in reasonable agreement with above two treatments, as shown in Fig. 1, giving a room-temperature value of 107 $cm^2 V^{-1} s^{-1}$. The inset of Fig. 1 shows the comparison of computing time of different methods under the same computational condition. It can be seen that the computing time of direct DFPT calculations is nearly two orders of magnitude larger than that using Wannier functions interpolation, although the initial **k** and **q** grids are merely increased from $12 \times 12 \times 1$ to $32 \times 32 \times 1$. The alternative choice is assuming 3D monolayer/superlattices, which saves a lot of computing time as compared to direct DFPT calculations but still spends much longer time than the 2D system due to the additional meshing dimension. Using a 2D Fröhlich model retains the high efficiency of the current Wannier functions interpolation framework of the 3D system, which is not surprising since only small changes are made in the long-range analytical model. From above, we can see that polar interaction in monolayer InSe is very strong. The 2D Fröhlich model has demonstrated its good ability in capturing the strong polar effect by giving reasonable results. We also calculated the electron mobility of monolayer MoS_2, which has relatively weak polar interaction (Fig. S7 in the supplementary material) and found that the 2D Fröhlich model still works well. Therefore, the 2D Fröhlich model can be recommended for the calculation of electrical transport of 2D polar materials in terms of balancing the calculational accuracy and computational consumption.

Although monolayer InSe possesses many fascinating properties such as high thermal stability and large bandgap, its electron mobility is not competitive in electronic applications as compared to other 2D materials. In polar materials, long-range Coulomb

interaction leads to the LO phonon and transverse optical (TO) phonon spitting in the long wavelength limit, and the spitting behavior is affected by the dimensionality.[27] In the 3D system, the degeneracy of LO and TO phonon modes at long wavelength limit is removed, whereas for the 2D system, the splitting depends on the phonon momentum and vanishes at the Brillouin zone center, as shown in Fig. 2(a). It can be seen that the polar effect is significant for the highest LO phonon branch, whereas the other branches remain unchanged. Figure 2(b) shows the scattering rates as a function of electron energy and phonon frequency. Not all phonons can participate in the scattering process of electrons imposed by the constraint of energy and momentum conservations. Since the electrons are located in the Γ valley (the inset of Fig. S5 in the supplementary material), the effective scattering phase space of phonons is mainly around Γ as can be seen from the phonon frequency dependence. Figure 2(b) clearly shows that the scattering of the highest LO phonons is much stronger than that of other branches, due to the strong Fröhlich coupling, which thus dominates the electron mobility. Therefore, suppressing the Fröhlich scattering in monolayer InSe would increase the mobility.

It has been revealed that the carrier mobility of the 2D system can be improved by modulating the dielectric environments around it due to the dielectric mismatch.[33,34] This effect can be well evaluated by the 2D Fröhlich model via changing the parameter of $\varepsilon^0_{\text{eff}}$. In an application like the hBN-encapsulated field-effect devices,[35] InSe is covered by dielectric materials and forms the 2D electron gases structure as shown in Fig. 3. If $\varepsilon^0_{\text{eff}}$ is set to be 4, close to the dielectric constant of hBN, the mobility is greatly enhanced, up to 361 $\text{cm}^2\,\text{V}^{-1}\,\text{s}^{-1}$ at room temperature. As the $\varepsilon^0_{\text{eff}}$ is further increased, the mobility attains more improvement, and the enhancement approaches saturation, since the scattering of LO phonons is no longer the dominance when the $\varepsilon^0_{\text{eff}}$ is high enough, as shown in Fig. 2(c). Notably, the mobility of monolayer InSe can be enhanced by 3–6 times in the temperature range of 100–600 K, reaching up to 525 $\text{cm}^2\,\text{V}^{-1}\,\text{s}^{-1}$ at room temperature.

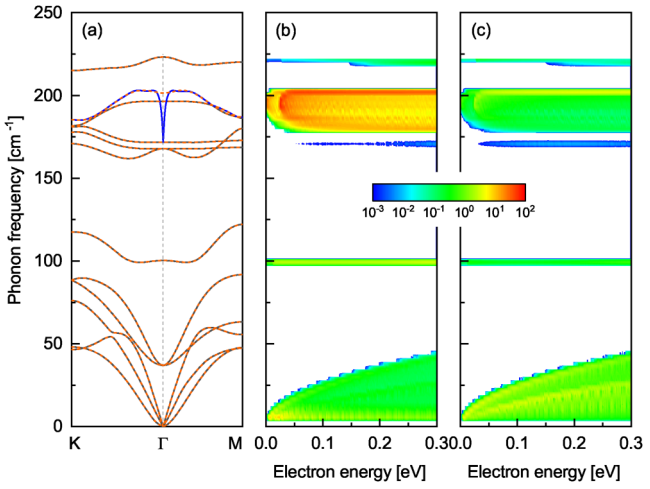

FIG. 2. (a) Phonon dispersion of monolayer InSe including polar correction based on 3D periodicity (dashed line), and 2D Coulomb cutoff (solid line) with the highest LO branch marked in blue. (b) Scattering rates as a function of electron energy and phonon frequency for freestanding monolayer InSe and (c) that of coated monolayer InSe covered by dielectric materials with a dielectric constant of 10.

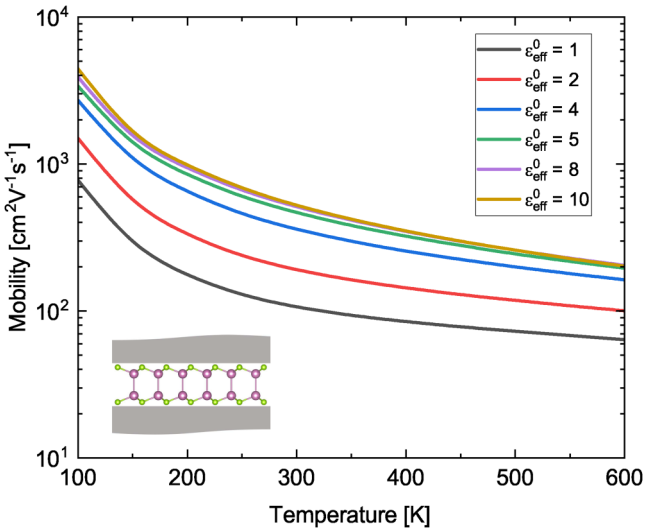

FIG. 3. Electron mobilities of monolayer InSe coated by materials with different dielectric constants.

IV. CONCLUSION

In summary, since Fröhlich interaction in the 2D system behaves differently from the 3D system, several approximate treatments are usually used; the accuracy of each is examined in this work by the first-principles calculations combined with the iterative solution of BTE in monolayer InSe. The electron mobility of monolayer InSe calculated without polar effect can be an order of magnitude larger than that calculated using the 3D Fröhlich model, indicating that Fröhlich interaction is significant and thus needs to be taken seriously. Therefore, by truncating the Coulomb interaction perpendicular to the basal plane, the monolayer InSe is purely isolated and thus 2D Fröhlich interaction is captured from the start of direct DFPT calculations; in this way, it is known that the electron mobility should be in the order of 100 $\text{cm}^2\,\text{V}^{-1}\,\text{s}^{-1}$ at room temperature. Another cunning calculation by treating the 2D system as 3D monolayer/vaccum supperlattices give close results. More importantly, the 2D Fröhlich analytical model with the screening dielectric effect has demonstrated its great ability by guaranteeing good results, at a drastically reduced computational cost due to its good compatibility in the current Wannier functions interpolation framework. In addition, the 2D Fröhlich model allows the quantitative evaluation of the modulating effect from the dielectric environment. It is found that the electron mobility of monolayer InSe can be considerably enhanced, up to 525 $\text{cm}^2\,\text{V}^{-1}\,\text{s}^{-1}$ at room temperature, by coating high dielectric materials due to the strong suppression of the Fröhlich interaction.

SUPPLEMENTARY MATERIAL

See the supplementary material for SERTA and iterative solutions of BTE, convergence check with respect to initial and final grids, mobility of monolayer InSe using LDA pseudopotentials, and calculations for monolayer MoS_2.

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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