Monolayers of transition-metal dichalcogenides (TMD) hold great promise as future nanoelectronic and optoelectronic devices. An essential feature for achieving high device performance is the use of suitable supporting substrates, which can strongly affect the electronic and optical properties of these two-dimensional (2D) materials. Here, we investigate the effect of substrate screening on the quasiparticle band structure of monolayer MoS$_2$ by performing many-body GW calculations with an effective dielectric screening. We show that the substrate can have a significant effect on the quasiparticle band gap, for example the gap renormalization is as large as 250 meV for MoS$_2$ on SiO$_2$. Within the $G_0W_0$ approximation, we find that the supported monolayer exhibits a direct band gap, in contrast to the free-standing monolayer. We also find that substrate screening induces an enhancement of the carrier effective masses by as much as 27% for holes, shifts plasmon satellites, and redistributes quasiparticle weight. Our results highlight the importance of the dielectric environment in the design of 2D TMD-based devices.
quasiparticle band structures in semiconductors. The method is based on the calculation of the electron self-energy, which includes exchange and correlation effects via the dynamically-screened Coulomb interaction. The screened Coulomb interaction \( W(r, r'; \omega) \) is most often calculated within the random-phase approximation (RPA), starting from Kohn-Sham wavefunctions obtained within density functional theory (DFT)\(^6\).

Standard implementations of the GW methods obtain the electron Green’s function and the RPA polarization by using an expansion over unoccupied Kohn-Sham states.\(^{61–63}\) Although very successful, in this approach the convergence with respect to unoccupied states is challenging, which results in a heavy computational load. To circumvent this bottleneck, several groups have been pursuing direct calculations of \( G \) and/or \( W \) using the Sternheimer equation or variants of this method\(^{62–63}\) in this work we employ the SternheimerGW method that we developed\(^69\), whereby both the screened Coulomb interaction and the electron Green’s function are evaluated using solely the occupied Kohn-Sham states. Below we briefly review this methodology. More details and the derivation of key equations can be found in Refs.\(^{69–71}\).

The Green’s function \( G(r, r'; \omega) \) and the screened Coulomb interaction \( W(r, r'; \omega) \) are expressed in terms of the space coordinate \( r' \), while \( r \) and \( \omega \) are treated as parametric space and frequency variables. The Green’s function is calculated by solving the inhomogeneous linear system of equations for all occupied states

\[
(H - \hbar \omega) G_{0[r, \omega]}(r') = -\delta_{r-r'}.
\]  

Here, \( H \) corresponds to the single-particle Kohn-Sham Hamiltonian and \( \delta \) is the Dirac delta function.

The screened Coulomb interaction \( W_0(r, r'; \omega) \) within the RPA\(^{62–63}\) can be obtained by the procedure outlined below. When the system is subject to a perturbation \( \Delta V_{[r, \pm \omega]}(r') \), the corresponding change in the charge density is given by

\[
\Delta n_{[r, \omega]}(r') = 2 \sum_{\nu} \psi_{\nu}^*(r') \left[ \Delta \psi_{\nu[r, +\omega]}(r') + \Delta \psi_{\nu[r, -\omega]}(r') \right],
\]  

where \( \Delta \psi_{\nu[r, \pm \omega]}(r') \) are the frequency-dependent variations of the occupied single-particle wavefunctions. These variations are obtained by solving the following Sternheimer equation

\[
(H - \epsilon_{\nu} \pm \hbar \omega) \Delta \psi_{\nu[r, \pm \omega]}(r') = -(1 - \bar{P}_v) \Delta V_{[r, \pm \omega]}(r') \psi_{\nu}(r').
\]  

The operator \( \bar{P}_v = \sum_{\nu} \psi_{\nu} \langle \psi_{\nu} \rangle \) projects onto the occupied manifold, and \( \epsilon_{\nu} \) are the corresponding Kohn-Sham energy eigenvalues. There are two methods of choosing the perturbation \( \Delta V_{[r, \pm \omega]}(r') \) that yield \( W_0(r, r'; \omega) \). In the direct (non-self-consistent) approach, the perturbation is set to the bare Coulomb potential \( \Delta V_{[r, \pm \omega]}(r') = v(r, r') \). From the variation in the charge density, the RPA dielectric function is evaluated as

\[
\varepsilon_{[r, \omega]}(r') = \delta_{r-r'} - \Delta n_{[r, \omega]}(r').
\]  

The screened Coulomb interaction \( W_0(r, r'; \omega) \) is then calculated by inverting \( \varepsilon \) via

\[
W_0[r, \omega](r') = \int dr'' v(r, r'') \varepsilon^{-1}(r'', r'; \omega).
\]  

In the self-consistent method, the perturbation is set to the screened Coulomb interaction \( \Delta V_{[r, \pm \omega]}(r') = W_0(r, r'; \omega) \). This scheme initializes the perturbation \( \Delta V_{[r, \pm \omega]}(r') \) to the bare Coulomb interaction \( v(r, r') \). Then, the induced variation in the charge density \( \Delta n_{[r, \omega]}(r') \) generates a Hartree potential that screens the bare Coulomb interaction through

\[
\Delta V_{[r, \omega]}(r') = \int dr'' \Delta n_{[r, \omega]}(r'') v(r'', r').
\]  

The updated screened Coulomb interaction \( W_0(r, r'; \omega) \), given by

\[
W_0[r, \omega](r') = v(r, r') + \Delta V_{[r, \omega]}(r'),
\]  

is subsequently used to evaluate the next density response. This process is iterated until convergence is reached.

The self-energy, \( \Sigma \), is obtained as the product of the Green’s function \( G_0 \) and the screened Coulomb interaction \( W_0 \)

\[
\Sigma(r, r'; \omega, \omega') = \frac{i}{2\pi} \int_{-\infty}^{+\infty} G_0(r, r'; \omega + \omega') W_0(r, r'; \omega') e^{-i\omega' d\omega'},
\]  

and the quasiparticle energies can thus be determined as

\[
\epsilon_{nk}' = \epsilon_{nk} + Z_{nk} \langle \psi_{nk} | \Sigma(\epsilon_{nk}) - V_{xc_{nk}} | \psi_{nk} \rangle,
\]  

where \( \epsilon_{nk}, \psi_{nk}, \) and \( V_{xc_{nk}} \) are, respectively, the Kohn-Sham DFT eigenvalues, wavefunctions, and the expectation value of the exchange-correlation potential of the \( n^{th} \) band. \( Z_{nk} = [1 - \langle \psi_{nk} |\partial \Sigma(\epsilon)/\partial \epsilon | e^{-\epsilon_{nk} \psi_{nk}} | \psi_{nk} \rangle]^{-1} \) is the quasiparticle renormalization factor that defines the quasiparticle weight carried by the excitation. The SternheimerGW method provides the possibility of calculating the complete energy- and momentum-resolved spectral function \( A(\omega, k) \), a physical observable that can be extracted from angle-resolved photoemission (ARPES) measurements. \( A(\omega, k) \) is calculated as

\[
A(\omega, k) = \frac{1}{\pi} \times \sum_{n} \frac{|\text{Im} \Sigma_{n}(\omega, k)|}{|\text{Re} \Sigma_{n}(\omega, k)|^2 + |\text{Im} \Sigma_{n}(\omega, k)|^2},
\]  

in which \( \text{Re} \Sigma \) and \( \text{Im} \Sigma \) indicate the real and imaginary parts of the \( G_0 W_0 \) self-energy, and \( \Delta \text{Re} \Sigma_{n}(\omega, k) = \text{Re} \Sigma_{n}(\omega, k) - V_{xc_{nk}} \).
FIG. 1: Schematic of a MoS$_2$ monolayer on an h-BN and an SiO$_2$ substrates. In the present work the substrate is modeled using an effective dielectric environment.

B. Computational details

Ground-state calculations are carried out using density functional theory as implemented in the Quantum ESPRESSO package. The Kohn-Sham wavefunctions and energies are calculated using the PBE functional. A plane-wave basis is used with energy and charge-density cutoffs of 50 Ry and 200 Ry, respectively. We approximate the core-valence interactions via norm-conserving pseudopotentials, explicitly including the 4s and 4p semicore electrons of Mo. The Brillouin Zone (BZ) integration is sampled using a $15 \times 15 \times 1$ Monkhorst-Pack k-point grid. The atomic positions are relaxed at the experimental lattice constant $a = 3.16$ Å. To avoid spurious interactions between periodically repeated slabs, the size of the computational cell, including monolayer and vacuum, is set to 20 Å in the out-of-plane direction, unless otherwise stated.

We perform $\text{G}_0\text{W}_0$ calculations starting from the PBE wavefunctions and energy eigenvalues. The dielectric matrix $\varepsilon$ is computed within the random phase approximation using either the Godby-Needs plasmon-pole approximation (PPA) with an imaginary pole energy of 16 eV, or using full frequency integration (FF), as implemented in the STERNHEIMERGW code. The FF integration is performed along the imaginary axis using 65 discrete frequencies in the interval of 0 eV to 240 eV. We obtain the FF self-energy on the real axis using an analytic continuation following the adaptive Antoulas-Anderson method.

C. Numerical convergence tests

For accurate results GW calculations require the convergence of several numerical parameters. In this section, we discuss the dependence of the band gap and the energy of the band extrema with respect to the energy cutoff for exchange and correlation, as well as the sampling of the Brillouin zone using the PPA.

To avoid spurious Coulomb interactions between electrons belonging to periodic images of the monolayer, we truncate the Coulomb interaction $v$, both in the calculation of the dielectric function, $\varepsilon$, and of the screened Coulomb interaction, $W = \varepsilon^{-1}v$. In particular, we employ a 2D truncation scheme in reciprocal space, using the expression of Refs. 81 and 82:

$$v_{2D}(k) = 4\pi[1 - \exp(-\sqrt{k_x^2 + k_y^2}L_z)\cos(k_zL_z)]/|k|^2.$$  

Here $L_z$ is the cutoff distance in the out-of-plane direction. At the DFT level, we truncate the bare Coulomb potential using the scheme of Ref. 83, which speeds up the convergence of the GW calculations with respect the Brillouin zone grid. We note that this truncation is important: without truncation the GW band gap would be underestimated by about 0.26 eV.

In order to take into account the effect of substrate polarization, we renormalize the screened Coulomb interaction by the effective background dielectric constant ($\varepsilon_{\text{eff}}$) through

$$\varepsilon_{\text{eff}} = (1 + \varepsilon_s)/2,$$

where $\varepsilon_s$ refers to the relative dielectric constant of the substrate. Using this approach we model two substrate materials, SiO$_2$ ($\varepsilon_s = 3.9$) and a monolayer or a few layers of h-BN ($\varepsilon_s = 2.6$). Fig. 1 shows a qualitative schematic of the systems that we model, however we emphasize that our calculations contain a single layer of MoS$_2$, without substrate atoms.

To study the convergence of $E_x$ we set a correlation cutoff $E_x = 15$ Ry (1 Ry = 13.605 eV); conversely, to study the convergence with respect to $E_x$, the exchange cutoff is set to $E_x = 45$ Ry. In both convergence tests, the BZ
FIG. 2: Difference (ΔE) of the quasiparticle band gap (QP gap), valence band maximum (VBM) and conduction band minimum (CBM) from the corresponding converged values, as a function of (a) exchange (Ex) and (b) correlation (Ec) self-energy cutoff. The values are obtained at the high symmetry K point. The difference between the last two values of the gap in (a) and (b) are 2 meV and 16 meV, respectively.

TABLE 1: Dependence of the quasiparticle band gap (QP gap), valence band maximum (VBM) and conduction band minimum (CBM) at the high symmetry K point on the number of q-points used to sample the BZ. The exchange (Ex) and correlation (Ec) self-energy cutoffs are set to 45 Ry and 15 Ry, respectively.

| q mesh | irreducible points | VBM (eV) | CBM (eV) | QP gap (eV) |
|--------|--------------------|----------|----------|-------------|
| 09 × 09 × 1 | 12 | −5.864 | −2.822 | 3.04 |
| 12 × 12 × 1 | 19 | −5.729 | −2.949 | 2.78 |
| 15 × 15 × 1 | 27 | −5.726 | −3.006 | 2.72 |
| 18 × 18 × 1 | 37 | −5.753 | −3.038 | 2.72 |
| 21 × 21 × 1 | 48 | −5.785 | −3.054 | 2.73 |

is sampled using a 15 × 15 × 1 q-point mesh (27 irreducible points) for the dielectric matrix and the screened Coulomb interaction. Fig. 2a shows that VBM and CBM are well converged for Ex above 35 Ry, increasing by only 12 meV when we increase the cutoff all the way to 45 Ry. Since both band extrema converge from the top at a similar rate, the QP gap converges much faster, and is accurate to within 2 meV already for Ex = 25 Ry. Fig. 2b shows that the convergence with respect to Ec is somewhat slower, but the changes in the VBM, CBM, and QP gap from Ec = 15 Ry to 16 Ry are of 15 meV, 31 meV, and 16 meV respectively. For Ec = 16 Ry, the QP gap is found to be 2.70 eV, which is remarkably (and probably coincidentally) the same value as reported in experiments on suspended layers. As in the present work, these previous calculations employ the experimental lattice parameter. Differences between reported band gaps arise from differences in the GW calculations, specifically the Coulomb truncation and the vacuum size. Despite such differences, our calculations also indicate that the G0W0 band gap of a pristine MoS2 monolayer is indirect. We do not include spin-orbit coupling in our calculations, because the resulting energy splittings at the K point amount to 3 meV (CBM) and 147 meV (VBM) at the DFT level, which is below the numerical precision of our GW calculations.

III. RESULTS AND DISCUSSION

A. Quasiparticle band gap and band structures

In this section we discuss our results for the quasiparticle band gap and band structure of monolayer MoS2 monolayer, as obtained by considering a layer in vacuum, the effective screening from a SiO2 substrate, and the effective screening resulting from h-BN. The following results correspond to exchange and correlation cutoffs Ex = 45 Ry and Ec = 15 Ry, and a 15 × 15 × 1 q-point grid. In Fig. 3a, we compare the DFT and the G0W0/PPA band structure of a MoS2 monolayer on a (virtual) SiO2 substrate. The G0W0 correction is not uniform throughout the Brillouin zone, so that not only the band gap but also the effective masses are modified (see Sec. III B). In Table 2, we compare the calculated QP gap, VBM, and CBM at the high-symmetry K point of the free-standing (FS) MoS2 monolayer, with a monolayer deposited on (virtual) h-BN or SiO2 substrates. When using full frequency integration, the band
extrema shift to lower energies, and the QP gap is reduced as compared to the PPA model. This reduction ranges from 40 meV for the FS monolayer to 80 meV for the monolayer on substrate.

We find that the substrate screening renormalizes the absolute quasiparticle energies of the VBM and CBM. As a consequence, the quasiparticle band gap is also reduced as compared to the free-standing monolayer. In particular, we find a reduction of the band gap by 180(140) meV when using FF(PPA) frequency integration for h-BN, and of 250(210) meV for SiO$_2$. This reduction is expected since the Coulomb energy required for adding/removing an electron in monolayer MoS$_2$ is reduced by the dielectric screening of the substrate.

In line with our finding, previous experimental and theoretical work indicates the sensitivity of the QP gap to the dielectric screening environment, as shown in Fig. 4. In the case of the SiO$_2$ substrate, scanning tunneling spectroscopy (STS) measurements obtain a QP gap of 2.1 eV. However, optical absorption measurements on the same sample used for STS in Ref. 31 yield a gap of 2.44 eV. This latter value agrees with our FF QP gap (2.43 eV) for monolayer MoS$_2$ on SiO$_2$. Ref. 31 argues that the tunneling gap is underestimated due to band-tail states near the conduction band minimum. Overall, the calculated band gaps from literature, which we reproduce in Fig. 4, are in qualitative agreement with experiments. However, the magnitude of the QP gap renormalization is generally underestimated. A particularly good agreement between theory and experiments is found for the MoS$_2$ monolayer on a h-BN substrate. The carefully converged GW QP gap (2.36 eV) of Ref. 17 is very similar to the QP gap measured by STS (2.35 eV) in Ref. 31. In our calculations, when we consider FF integration and $\varepsilon_s = 5.9$ corresponding to the dielectric constant of bulk h-BN, We obtain a QP gap of 2.35 eV, which is in excellent agreement with the above theoretical and experimental values.

One interesting result of our calculations is that the screening of the substrate changes the character of the QP gap. As mentioned above, $G_0W_0$ predicts an indirect QP gap for the free-standing MoS$_2$ monolayer at the experimental lattice parameter (3.16 Å). The substrate-induced renormalization induces a direct QP gap, both in the case of SiO$_2$ and h-BN screening. Fig. 3 illustrates this change in between the free-standing monolayer and a monolayer in the presence of dielectric screening from an SiO$_2$ substrate. In the presence of substrate screening, the CBM at the midpoint, Q, of the high-symmetry Γ–K path (see Fig. 3) raises above the CBM at the K point as compared to the unscreened case. Introducing the energy difference $\Delta = CBM_K - CBM_Q$, we find $\Delta_{FS} = 98$ meV, $\Delta_{hBN} = 57$ meV, and $\Delta_{SiO2} = -94$ meV using the FF method. In the PPA calculations these differences are less pronounced: $\Delta_{FS} = 65$ meV, $\Delta_{hBN} = 15$ meV, and

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**TABLE 2:** Quasiparticle band gap (QP gap, eV), valence band maximum (VBM) and conduction band minimum (CBM) at the high-symmetry K point, for the free-standing (FS) MoS$_2$ monolayer, and for the same layer in the dielectric environment corresponding to an h-BN or a SiO$_2$ substrate.

| Substrate | VBM | CBM | QP gap |
|-----------|-----|-----|--------|
| FS        | PPA | FF  | PPA | FF |
| h-BN      | PPA | FF  | PPA | FF |
| SiO$_2$   | PPA | FF  | PPA | FF |
FIG. 4: Quasiparticle band gap of a MoS$_2$ monolayer on different substrates reported in the literature. The experimental results in blue circles are obtained with scanning tunneling microscopy/spectroscopy (STM/STS) absorbance, and angle-resolved (inverse) photoemission spectroscopy (ARPES/ARIPES). The GW band gaps are shown with the orange circles. The horizontal lines represent our calculated quasiparticle gaps using FF integration for the FS monolayer, and for h-BN and SiO$_2$ screening.

$\Delta_{\text{SiO}_2} = -60$ meV. This indicates that the screening-induced renormalization is more significant at the K point, and especially so when using FF integration. Unlike the CBM, the maximum of the valence band remains at the K point irrespective of substrate screening. The energy difference $\Delta_{\text{VBM}}$ between the VBMs at the K and $\Gamma$ point are 0.23 eV, 0.19 eV and 0.17 eV for the FS, the h-BN-screened, and the SiO$_2$-screened monolayer, respectively. Again the PPA yields smaller differences, in the range of 0.20–0.30 meV. It should be noted that self-consistent GW calculations are necessary for predicting a direct band gap as observed in photoluminescence measurements.

Overall, the present results show that the dielectric environment alters qualitatively and quantitatively the QP gap of monolayer MoS$_2$. It is natural to expect the same behavior for other monolayer TMDs.

B. Electron and hole effective-masses

The effective masses $m^* = \hbar^2 (\partial^2 E/\partial k^2)^{-1}$ of electrons and holes at the K point are calculated along the high-symmetry K–$\Gamma$ and K–M lines. We evaluate the second derivatives of the band curvatures numerically, using a step $\Delta k = 0.01$ Å$^{-1}$ around the K point. Since in the Sternheimer-GW method the Green’s function and the screened Coulomb interaction are computed separately, we can directly determine quasiparticle energies $E_k$ for arbitrary k-points, without using interpolation techniques. Our calculated effective masses are shown in Table 3. The electron and hole effective masses obtained within DFT are 0.43 $m_0$ and 0.52 $m_0$, respectively, consistent with previously reported values $\approx 0.40$ $m_0$. The GW effective masses for the free-standing MoS$_2$ monolayer are in a good agreement with previous GW data available in the literature, in the range of 0.35–0.40 $m_0$ for electrons and 0.39–0.49 $m_0$ for holes. In the presence of substrate screening, the effective masses are heavier than for the FS layer.

We find that, for the h-BN (SiO$_2$) substrate, the electron effective mass $m_e$ is enhanced by 5% (8%) whereas the hole effective mass $m_h$ increases by 17% (27%) with respect to the FS layer. As for the quasiparticle shifts, the effective mass enhancement due to the screening is more pronounced for calculations performed FF integration rather than the PPA.

Effective masses have been measured for a MoS$_2$ monolayer separated from a MoS$_2$ bulk compound by intercalating potassium using angle-resolved photoemission spectroscopy (ARPES). The extracted effective
TABLE 3: Calculated electron and hole effective masses of the free-standing (FS) and substrate-screened MoS$_2$ monolayer at the K point.

| Substrate   | m$_e$/m$_0$ | m$_h$/m$_0$ |
|-------------|-------------|-------------|
| FS          | 0.39        | 0.43        |
| h-BN        | 0.40        | 0.43        |
| SiO$_2$     | 0.40        | 0.43        |

masses at the K point are $m_e = (0.67 \pm 0.08) m_0$ and $m_h = (0.60 \pm 0.08) m_0$. These values are significantly higher than in our calculations and previous theoretical work. The difference could originate from the heavy doping of the conduction band with electrons by the potassium intercalation, which would induce metallic screening. This interpretation is consistent with the fact that the gap extracted from ARPES is $1.86 \pm 0.02$ eV, which is significantly smaller than other measured optical gaps and calculated quasiparticle gaps (see Refs. 103, 105). Here, the spectral function $A(\omega, k)$ is given by $A(\omega, k) = \int d\omega_{\text{p}} g(\omega_{\text{p}}) \delta(\omega - \omega_{\text{p}})$. The inset of Fig. 4 clearly shows a plasmon satellite at around $22$ eV, arising from the excitation of the high-energy $\pi + \sigma$ plasmons. On the other hand, the low-energy $\pi$ plasmons are not visible; these features possibly overlap with the broad main quasiparticle peaks. We emphasize that the energy and intensity of these plasmonic satellites are not captured correctly by $B_0 W_0$, which are known to overestimate the binding energy of satellites. For an accurate description of these features one would need to perform cumulant expansion calculations. Earlier studies of plasmon satellites of TMDs within the cumulant expansion method can be found in Ref. 114.

Our calculated reduced electron-hole effective masses, $m_e = m_e m_h/(m_e + m_h)$, for the free-standing monolayer and for h-BN or SiO$_2$ screening, are $0.20 m_0$, $0.22 m_0$, and $0.23 m_0$, respectively. These values should be compared with the measured exciton’s reduced mass $m_t = 0.27 m_0$, as obtained from magneto-optical spectroscopy experiments. The slight difference may be due to the fact that, in the experiment, the MoS$_2$ monolayer is encapsulated between slabs of h-BN, therefore the screening is enhanced as compared to our calculations.

C. Self-energy and spectral function

In this section, we discuss the effect of substrate screening on the electron self-energy, the spectral function, and the related incoherent plasmonic structure. For these calculations it is necessary to employ FF integration as opposed to the PPA. Figs. 5a-d show the frequency-dependent real and imaginary parts of the self-energy of the VBM and the CBM at the K point, both for the free-standing and substrate-screened monolayer MoS$_2$. The real part determines the quasiparticle shift and renormalization, the imaginary part determines the quasiparticle broadening and lifetimes. We can see that both Re$(\Sigma)$ and Im$(\Sigma)$ have a pronounced structure in the range of 15–25 eV, which arises from plasmon excitations. In fact, the electron loss spectra of MoS$_2$ monolayer exhibit the characteristic of low-energy and high-energy plasmon resonances called $\pi$ and $\sigma$ at 7.6 eV and 15.6 eV, respectively, which arise from the collective excitation of the $(\text{Mo})d$ and $(\text{S})s, p$ states. Here, the spectral function $A(\omega, k)$ in Figs. 5f clearly shows a plasmon satellite at around $22$ eV, arising from the excitation of the high-energy $\pi + \sigma$ plasmons. On the other hand, the low-energy $\pi$ plasmons are not visible; these features possibly overlap with the broad main quasiparticle peaks. We emphasize that the energy and intensity of these plasmonic satellites are not captured correctly by $B_0 W_0$, which are known to overestimate the binding energy of satellites. For an accurate description of these features one would need to perform cumulant expansion calculations. Earlier studies of plasmon satellites of TMDs within the cumulant expansion method can be found in Ref. 114.

IV. CONCLUSIONS

In summary, we investigated the dielectric screening effect of a substrate on the quasiparticle properties of monolayer MoS$_2$ using the first-principles SternheimerGW method. We showed that substrate polarization reduces the quasiparticle band gap by as much as...
FIG. 5: (a)-(b) Real part of the $G_0W_0$ self-energy ($\Sigma$) of monolayer MoS$_2$ for the VBM and CBM states. (c)-(d) Corresponding imaginary part of the self energy. (e)-(f) Corresponding spectral functions $A(\omega, k)$. All calculations are performed at the K point for the free-standing monolayer (FS; black), the case with h-BN screening (red), and the case with SiO$_2$ screening (blue).

$G_0W_0$ calculations yield an indirect fundamental band gap for the free-standing MoS$_2$ monolayer, using the experimental lattice parameters. Here, we found that in the presence of substrate screening, the $G_0W_0$ band gap exhibits a direct character. This result is independent of the frequency integration scheme (FF or PPA). The sensitivity of the direct/indirect character of the gap to substrate screening is a new element to be taken into account when using ab initio many-body calculations to predict the optoelectronic properties of 2D materials.

We also found that substrate screening affects the dispersions of quasiparticle bands. For example, screening enhances the electron and hole carrier effective masses at the K point are enhanced by as much as 8% and 27%, respectively. The resulting masses are in very good agreement with experiments.

An analysis of the $G_0W_0$ self-energy and spectral function reveals that these results can be rationalized in terms of the shift of the plasma resonances as a result of the changing dielectric environment, in line with a simple Drude model of plasmon excitations.

On the methodology side, the calculations of interpolation-free quasiparticle effective masses and of spectral functions illustrate some of the capabilities of the SternheimerGW approach, and provide further vali-
dation of this emerging methodology.

Our present findings provide new insight into the role of the dielectric environment in the quasiparticle band structure of the prototypical TMD monolayer MoS2. More generally, our work suggests that substrate engineering could offer new avenues to design future TMD-based electronic and optoelectronic devices.

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