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Plasmon and quasiparticle band structures in β -SiC

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We use a recently developed plasmon-pole model to calculate the plasmon band structure in β -SiC. The obtained lowest plasmon energy is in excellent agreement with electron-energy-loss measurements. We also employ this plasmon-pole model for an analytic description of the energy dependence of the dynamically screened interaction W , which is used to calculate the quasiparticle band structure in the GW approximation. This band structure compares favorably with experiment and with other calculations using different techniques.

I. PLASMON BAND STRUCTURE

Recently, Engel and Farid¹ developed a plasmon-pole model that not only provides an analytic description of the energy dependence of the various dielectric response functions of a crystalline material, but also yields a real valued plasmon band structure that has a physical meaning and that can be compared with experiment. This in contrast to several other plasmon-pole models known to us,²⁻⁵ in which the plasmon poles are not supposed to have any physical meaning. The plasmon energies $\omega_m(\mathbf{q})$ as a function of reciprocal lattice vector $\mathbf{q}$ in this model are obtained from the following generalized eigenvalue problem:

$$\underline{\chi}(\mathbf{q}, \epsilon = 0) \vec{x}_{m,\mathbf{q}} = -\frac{1}{\omega_m^2(\mathbf{q})} \underline{M}(\mathbf{q}) \vec{x}_{m,\mathbf{q}}, \quad (1)$$

where $\underline{\chi}(\mathbf{q}, \epsilon = 0)$ is the full static polarizability matrix, with matrix elements $\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q}, \epsilon = 0)$ ($\mathbf{G}$ and $\mathbf{G}'$ are reciprocal lattice vectors), and $\underline{M}(\mathbf{q})$ is a matrix given by

$$M_{\mathbf{G},\mathbf{G}'}(\mathbf{q}) = \frac{\epsilon_{\text{pl}}^2}{4\pi\epsilon^2} (\mathbf{q} + \mathbf{G}) \cdot (\mathbf{q} + \mathbf{G}') \frac{\rho(\mathbf{G} - \mathbf{G}')}{\rho(0)}. \quad (2)$$

Here $\rho(\mathbf{G})$ are the Fourier components of the electron density and $\epsilon_{\text{pl}} = \hbar\sqrt{4\pi e^2 \rho(0)/m}$ is the plasma energy of a homogeneous electron gas with charge density $\rho(0)$. If the eigenvectors $\vec{x}_{m,\mathbf{q}}$ of Eq. (1), with components $x_{m,\mathbf{q}}(\mathbf{G})$, are normalized according to $\vec{x}_{m,\mathbf{q}}^\dagger \underline{M}(\mathbf{q}) \vec{x}_{n,\mathbf{q}} = \delta_{m,n}$, then the model full polarizability¹

$$\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q}, \epsilon) = \sum_m \frac{z_{m,\mathbf{q}}(\mathbf{G}) z_{m,\mathbf{q}}^*(\mathbf{G}')}{2\omega_m(\mathbf{q})} \times \left\{ \frac{1}{\epsilon - \omega_m(\mathbf{q}) + i\eta} - \frac{1}{\epsilon + \omega_m(\mathbf{q}) - i\eta} \right\} \quad (3)$$

satisfies the f -sum rule,⁶ and has the correct static

value. In this expression $\vec{z}_{m,\mathbf{q}} = \underline{M}(\mathbf{q}) \vec{x}_{m,\mathbf{q}}$ and η is an infinitesimally small positive energy. The full polarizability $\underline{\chi}(\mathbf{q}, \epsilon)$ is related to the irreducible polarizability $\underline{P}(\mathbf{q}, \epsilon)$ by $\underline{\chi}(\mathbf{q}, \epsilon) = \underline{P}(\mathbf{q}, \epsilon) [\underline{1} - \underline{v}(\mathbf{q}) \underline{P}(\mathbf{q}, \epsilon)]^{-1}$, where $\underline{v}(\mathbf{q})$ is the bare Coulomb interaction, $v_{\mathbf{G},\mathbf{G}'}(\mathbf{q}) = 4\pi e^2 \delta_{\mathbf{G},\mathbf{G}'} / |\mathbf{q} + \mathbf{G}|^2$, and $\underline{1}$ denotes the unit matrix $\delta_{\mathbf{G},\mathbf{G}'}$.

Since $\underline{\chi}(\mathbf{q}, 0)$ is a Hermitian and negative definite matrix, whereas $\underline{M}(\mathbf{q})$ is Hermitian and positive definite,¹ the eigenvalue problem defines real-valued plasmon frequencies $\omega_m(\mathbf{q})$, which we take positive. Calculations for Si have shown that the two lowest plasmon bands obtained with this model compare favorably with experiment.¹

In Fig. 1 we have plotted the lowest lying plas-

FIG. 1. The calculated dispersion of the lowest plasmon bands along the Δ and the Λ axes by the generalized eigenvalue problem for β -SiC.

mon bands for β -SiC (zinc blende) as obtained from Eq. (1) along the two most symmetric directions in the first Brillouin zone. For the irreducible polarizability $\underline{P}(\mathbf{q}, \epsilon)$ we used the random-phase approximation (RPA) expression,^{7,8} with energies and wave functions obtained from a local-density approximation (LDA) calculation. Our LDA calculation for β -SiC was self-consistently carried through in a plane wave basis of 609 plane waves (52 Ry). We used the experimental lattice constant of 4.36 Å. The implemented parametrization of the ionic *ab initio* norm-conserving pseudopotentials is the construction of Bachelet *et al.*¹⁰ The exchange potential was represented by the Kohn-Sham form with the Wigner interpolation formula for the correlation potential. The number of plane waves taken into account in the calculation of all the dielectric response functions was 229. The Brillouin zone integration appearing in the RPA expression for $\underline{P}(\mathbf{q}, 0)$ was replaced by a summation over a regular grid of $\mathbf{k}$ points. The plasmon bands plotted in Fig. 1 were fully converged taking only 216 $\mathbf{k}$ points (16 points in the irreducible wedge), except for the results at the Γ point, for which we needed approximately 3000 $\mathbf{k}$ points (149 points in the irreducible wedge). The lowest plasmon energy, which occurs at the Γ point, is calculated as 22.4 eV, which is in very good agreement with an electron-energy-loss measurement of 22.1 eV.⁹ We are not aware of any measurements of the plasmon dispersion away from the Γ point. It would be interesting to compare such measurements with our predictions.

We also calculated the static electronic macroscopic dielectric constant, defined as $\epsilon_M = 1/\epsilon_{\mathbf{G}=0, \mathbf{G}'=0}^{-1}(\mathbf{q} \rightarrow 0, \epsilon = 0)$, where the (symmetrized) inverse di-

electric matrix is given by $\epsilon_{\mathbf{G}, \mathbf{G}'}^{-1}(\mathbf{q}, \epsilon) = \delta_{\mathbf{G}, \mathbf{G}'} + 4\pi e^2 \chi_{\mathbf{G}, \mathbf{G}'}(\mathbf{q}, \epsilon) / (|\mathbf{q} + \mathbf{G}| |\mathbf{q} + \mathbf{G}'|)$. The value we calculated is $\epsilon_M = 6.85$, which is in good agreement with the experimental value of 6.5 in Ref. 11 and another recently calculated value of 6.7.⁵

II. QUASIPARTICLE BAND STRUCTURE

The plasmon model of Engel and Farid also allows very efficient *GW* calculations of quasiparticle energies. Since the *GW* quasiparticle wave functions are practically undistinguishable from the LDA wave functions,² which we also explicitly checked for β -SiC, it is sufficient to calculate the expectation value of the self-energy matrix for the LDA wave functions. The difference between the LDA and *GW* energies can accurately be accounted for in a first-order Taylor expansion of the self-energy around the LDA energies.² The screened interaction $\underline{W}(\mathbf{q}, \epsilon)$ can be written as

$$\begin{aligned} \underline{W}(\mathbf{q}, \epsilon) &= \underline{v}(\mathbf{q}) + \underline{v}(\mathbf{q}) \underline{\chi}(\mathbf{q}, \epsilon) \underline{v}(\mathbf{q}) \\ &\equiv \underline{v}(\mathbf{q}) + \underline{W}^{\text{scr}}(\mathbf{q}, \epsilon). \end{aligned} \quad (4)$$

Together with Eq. (3) this leads to a plasmon-pole description for $\underline{W}(\mathbf{q}, \epsilon)$, which allows analytic integration of the energy integral occurring in the *GW* expression for the self-energy.¹ The first term in Eq. (4) leads to the energy independent Fock contribution $\underline{\Sigma}^{\text{Fock}}(\mathbf{q}, \epsilon)$ to the self-energy $\underline{\Sigma}(\mathbf{q}, \epsilon)$. The second term, the screening part, leads to an energy dependent contribution $\underline{\Sigma}^{\text{scr}}(\mathbf{q}, \epsilon)$. The expectation value of this contribution is

FIG. 2. The calculated band structure for β -SiC along the Δ and the Λ axes within the LDA (dotted line) and the *GW* method (solid line).

TABLE I. The LDA and the quasiparticle energies (eV) for β -SiC.

$\mathbf{k}$	LDA	Present	RKP ^a	Expt. ^b
Γ_{1v}	-15.07	-16.13	-16.44	
Γ_{15v}	0.00	0.00	0.00	0.00
Γ_{1c}	6.57	7.81	7.35	
Γ_{15c}	7.24	8.66	8.35	7.75
X_{1v}	-10.12	-11.19	-11.24	
X_{3v}	-7.70	-8.38	-8.64	
X_{5v}	-3.06	-3.42	-3.62	-3.6
X_{1c}	1.22	2.37	2.34	2.390
X_{3c}	4.14	5.55	5.59	5.5, 4.7
X_{5c}	13.93	16.05	15.78	
L_{1v}	-11.57	-12.65	-12.75	
L_{1v}	-8.45	-9.15	-9.42	
L_{3v}	-0.98	-1.11	-1.21	-1.16
L_{1c}	5.46	6.76	6.53	4.2
L_{3c}	7.12	8.68	8.57	8.5
L_{1c}	10.14	12.08	12.04	

^aReference 5.

^bReference 11.

$$\langle n, \mathbf{k} | \Sigma^{\text{scr}}(\mathbf{k}, \epsilon) | n, \mathbf{k} \rangle = \frac{1}{(2\pi)^3 \hbar} \int_{\text{BZ}} d^3 q \sum_{l, m} \frac{\left| \sum_{\mathbf{G}} w_{m, \mathbf{q}}^*(\mathbf{G}) \sum_{\mathbf{G}'} d_{l, \mathbf{q}-\mathbf{k}}(\mathbf{G}') d_{n, \mathbf{k}}(\mathbf{G}-\mathbf{G}') \right|^2}{\epsilon - \epsilon_l(\mathbf{k}-\mathbf{q}) + [\omega_m(\mathbf{q}) - i\eta] \text{sgn}(\mu - \epsilon_l(\mathbf{k}-\mathbf{q}))}, \quad (5)$$

where $|n, \mathbf{k}\rangle$ denotes the LDA eigenstate and where μ is the chemical potential. This expression and its energy derivative have to be evaluated at the LDA energies $\epsilon = \epsilon_n(\mathbf{k})$. The coefficients $d_{l, \mathbf{q}}(\mathbf{G})$ are the plane wave coefficients of the LDA wave functions and the coefficients $w_{m, \mathbf{q}}(\mathbf{G})$ are related to the eigenvectors $\vec{x}_{m, \mathbf{q}}$ through $\vec{w}_{m, \mathbf{q}} = \nu(\mathbf{q}) \underline{M}(\mathbf{q}) \vec{x}_{m, \mathbf{q}} / \sqrt{2\omega_m(\mathbf{q})}$. We note that Eq. (5) leads to real quasiparticle energies in a broad region around the gap of the order of the minimum plasmon energy of 22.4 eV.

We would like to draw attention to the numerical efficiency with which Eq. (5) can be evaluated. In particular, the structure of the numerator as the square of the inner product of the vector $\vec{w}_{m, \mathbf{q}}$ with the convolution of $\vec{d}_{l, \mathbf{q}-\mathbf{k}}$ and $\vec{d}_{n, \mathbf{k}}$ and the fact that the plasmon poles do not depend on the reciprocal lattice vectors allow a very fast algorithm. Furthermore, the convolution can be performed with a fast Fourier transform algorithm.

Figure 2 displays our calculated quasiparticle band structure. The indirect band gap is calculated to be 2.37 eV and the lowest conduction state is located exactly at the X point. In Table I we give the LDA energies and our quasiparticle energies at high symmetry points in the first Brillouin zone, together with recently calculated values by Rohlfling *et al.*⁵ and some known experimental values. For the Brillouin integration in Eq. (5) we used a grid of 64 $\mathbf{k}$ points. The number of reciprocal lattice vectors

and bands taken into account was 229. With these values the quasiparticle energy differences were converged within 0.05 eV. The main differences between the present work and the work of Rohlfling *et al.*⁵ is the use of a different plasmon-pole model, different ionic pseudopotentials, and Gaussian orbitals as basis functions in that work.

The agreement between our calculated quasiparticle energies, the experimental values and the quasiparticle energies calculated by Rohlfling *et al.*⁵ is on the whole very good. Like these authors we mention the disagreement between the experimental and calculated electron energies $E(L_{1c})$ and $E(\Gamma_{15c})$. New measurements could decide whether the failure is on the theoretical or the experimental side.

We finally note that the so-called “scissor” operator works rather well in β -SiC. The uniform quasiparticle correction 1.13 eV, as calculated by Käckell *et al.*,¹² agrees within 0.2 eV with our full *GW* results throughout the Brillouin zone.

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