User Manual - WanTiBEXOS: a Wannier based Tight Binding code for electronic band structure, excitonic and optoelectronic properties of solids

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1 Introduction

WanTiBEXOS code is a computational tool which was written in Fortran90 and parallelized with OpenMP. Based on the Tight-Binding Hamiltonian created by Wannier90 code,[1], it was developed to study electronic band structures, optical properties including excitonic phenomena and topological characteristics of 0D, 1D, 2D and 3D materials. It has the following features:

- Band structure,

- DoS, Spin-DoS and Projected DoS,

- Berry Curvature (non-metallic systems only),

- Several options of Coulomb potentials designed for 3D, 2D and 0D systems,

- BSE solver using TDA approximation,

- Exciton band structure,

- Exciton wavefunctions,

- Exciton Radiative lifetimes

- Dielectric function and optical properties, with and without excitonic effects.

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program; if not, write to the Free Software Foundation, Inc., 51 Franklin Street, Fifth Floor, Boston, MA 02110-1301, USA.

2 Installation

To compile this code you need to have installed in your computer OpenMP, Intel Fortran compiler and Math Kernel Library (MKL). For VASP users, it's recommended to use the patch for generating the MLWF,[2] available in: `https://github.com/Chengcheng-Xiao/VASP2WAN90_v2_fix`. After install the necessary libraries, you can follow these steps to install the code:

1. Download the code at: `https://github.com/ac-dias/WanTiBEXOS`

2. Enter in the code folder,

3. Edit the makefile if necessary,

4. Open Linux terminal in code folder and write: `make all`,

5. All executable files will be at the bin folder.

2.1 Executable files

After compiling the code, seven executable files at bin folder will be generated. Each of them has the following functions:

- `wtb.x` : It is main executable file. It can be executed, using the following command: `wtb.x < input.dat`, where the `input.dat` file is the main input file, Warning: This code doesn't contain an interface with MPI, so do not try to run it using mpirun -np command.

- `wtbf.x` : It is faster than `wtb.x`. However it consumes more RAM memory in BSE calculations.

- `dirgapf.x` : This post processing script reads `band.dat` file and finds both direct and indirect bandgaps. It can be executed by following command: `dirgapf.x nb nocp nk < bands.dat > dirgap.out`, where `nb`, `nocp` and `nk` are the numbers of wannier projections, of occupied states and of **k**-points used to generate `band.dat` file, respectively.

- `param_gen.x` or `param_gen_vasp.x` : It's used as a pre processing tool to read wannier90.win and its output files, and then generates the MLWF-TB parameter's file named as `tb_hr.dat`. It should be executed in the folder containing DFT and Wannier90 outputs. Before running this script, the Wannier90 input.win file needs to be called `wannier90.win`.

- `nc_nv_finder.x` : This post processing tool could be used to estimate the number of conduction and valence states (`NBANDSC` and `NBANDSV`), necessary to provides a reliable dielectric function in the interval of `ENSPECI` to `ENSPECF`, writting this in the main input file. Run by the command: `nc_nv_finder.x < input.dat >> input.dat`.

3 Theoretical Formalism

The orthogonal tight-binding Hamiltonian, $H(\mathbf{k})$, obtained via the Wannier90 framework,[1] can be written as follows,

$$H(\mathbf{k}) = H_0 + \sum_{i=1}^{N} e^{i\mathbf{k}\cdot\mathbf{R_i}} H_{\mathbf{R_i}} \,, \tag{1}$$

where H_0 corresponds to the Hamiltonian in unit cell, which contains the on-site energies and hopping parameters inside the cell. $H_{\mathbf{R_i}}$ corresponds to the hopping matrices, representing the interaction between unit cell and neighbors cells, while the matrix elements of H_0 and $H_{\mathbf{R_i}}$ are the output from the Wannier90 package,[1] and the number of neighbors cell proportional to the **k**-mesh used for Wannier interpolation. In our code the values of H_0 and $H_{\mathbf{R_i}}$ are declared in the PARAMS_FILE.

The electronic energy levels are obtained as the following:

$$H(\mathbf{k})|n,\mathbf{k}\rangle = E_{n,\mathbf{k}}|n,\mathbf{k}\rangle \tag{2}$$

where $E_{n,\mathbf{k}}$ and $|n,\mathbf{k}\rangle$ are the eigenvalues and eigenvectors respectively, n corresponds to the band index, that could be addressed as v for the valence (occupied) states and c for the conduction (unoccupied) states, $\mathbf{k}$ are the $\mathbf{k}$-point in Brillouin zone.

3.1 Optical Properties

To obtain the optical properties, we calculated the real and imaginary parts of the frequency dependent dielectric tensor, $\varepsilon_{1,\alpha,\beta}(\omega)$ and $\varepsilon_{2,\alpha,\beta}(\omega)$, respectively, through the following expressions:

$$\varepsilon_{1,\alpha,\beta}(\omega) = \delta_{\alpha,\beta} + \frac{e^2 S_p}{\varepsilon_0 \Omega N_{\mathbf{k}}} \sum_{\mathbf{k},c,v} F_{\alpha,\beta}^{c,v,\mathbf{k}} \frac{(E_{c,\mathbf{k}} - E_{v,\mathbf{k}}) - \hbar\omega}{(\hbar\omega - (E_{c,\mathbf{k}} - E_{v,\mathbf{k}}))^2 + \eta^2} , \tag{3}$$

$$\varepsilon_{2,\alpha,\beta}(\omega) = \frac{e^2 S_p}{\varepsilon_0 \Omega N_{\mathbf{k}}} \sum_{\mathbf{k},c,v} F_{\alpha,\beta}^{c,v,\mathbf{k}} \frac{\eta}{(\hbar\omega - (E_{c,\mathbf{k}} - E_{v,\mathbf{k}}))^2 + \eta^2} , \tag{4}$$

where $\delta_{\alpha,\beta}$ is a delta kroenecker, S_p is the spin factor, being 1 for SOC and spin polarized calculations and 2 for non-polarized calculations, $F_{\alpha,\beta}^{c,v,\mathbf{k}}$, in the scope of independent particle approximation (IPA), corresponds to the oscillator force, defined by:

$$F_{\alpha,\beta}^{c,v,\mathbf{k}} = \frac{\langle c,\mathbf{k}|P_\alpha|v,\mathbf{k}\rangle\langle v,\mathbf{k}|P_\beta|c,\mathbf{k}\rangle}{(E_{c,\mathbf{k}} - E_{v,\mathbf{k}} - i\eta_1)(E_{c,\mathbf{k}} - E_{v,\mathbf{k}} + i\eta_1)} , \tag{5}$$

where Ω is the volume of unit cell, ε_0 is the vacuum permittivity constant, $N_{\mathbf{k}}$ is the number of $\mathbf{k}$-points employed for the BZ integration, ω is the incident photon frequency, $c(v)$ corresponds to the conduction(valence) states. η is a parameter to smooth the dielectric function, where $\eta = \eta_1 + \eta_2$, being η_1 defined by the input flag CSHIFT and η_2 automatically defined by the

code through the separation energy between the transition states. α and β corresponds to the components x, y and z in the dielectric tensor. P_α corresponds to the light-matter interaction operator, which is given by,

$$P_\alpha = \frac{\partial H(\mathbf{k})}{\partial k_\alpha} \, , \tag{6}$$

where $H(\mathbf{k})$ corresponds to the electronic Hamiltonian, and $\alpha = x, y, z$. For circularly polarized light, selected by the flag CPOL= T, the light-matter interaction operator for $\sigma_\pm$ are written by the following expression:

$$P_{\sigma_\pm} = \frac{1}{\sqrt{2}} \left(\frac{\partial H(\mathbf{k})}{\partial k_x} \pm i \frac{\partial H(\mathbf{k})}{\partial k_y} \right) \, . \tag{7}$$

It's well known the relation between the complex dielectric constant $\varepsilon(\omega)$ and the complex refractive index $\tilde{n}(\omega) = n(\omega) + i\kappa(\omega)$, where $n(\omega)$ is the refractive index and $\kappa(\omega)$ the extinction coefficient. They are related by:

$$\varepsilon(\omega) = \tilde{n}^2(\omega) \, , \tag{8}$$

separating $\varepsilon(\omega)$ in real and imaginary part, $\tilde{n}(\omega)$ in refractive index and extinction coefficient we have:

$$\varepsilon_{1,\alpha,\beta}(\omega) + i\varepsilon_{2,\alpha,\beta}(\omega) = n_{\alpha,\beta}^2(\omega) + 2in_{\alpha,\beta}(\omega)\kappa(\omega) - \kappa_{\alpha,\beta}^2(\omega) \, . \tag{9}$$

Then, we obtain the real and imaginary part of dielectric function, i.e.,

$$\varepsilon_{1,\alpha,\beta}(\omega) = n_{\alpha,\beta}^2(\omega) - \kappa_{\alpha,\beta}^2(\omega) \, , \tag{10}$$

$$\varepsilon_{2,\alpha,\beta}(\omega) = 2n_{\alpha,\beta}(\omega)\kappa_{\alpha,\beta}(\omega) \, . \tag{11}$$

From these two equations we derive the expressions of the extinction coefficient and of the refractive index, as follows,

$$\kappa_{\alpha,\beta}(\omega) = \left[\frac{\sqrt{\varepsilon_{1,\alpha,\beta}^2(\omega) + \varepsilon_{2,\alpha,\beta}^2(\omega)} - \varepsilon_{1,\alpha,\beta}(\omega)}{2} \right]^{\frac{1}{2}} \tag{12}$$

$$n_{\alpha,\beta}(\omega) = \left[\frac{\sqrt{\varepsilon_{1,\alpha,\beta}^2(\omega) + \varepsilon_{2,\alpha,\beta}^2(\omega)} + \varepsilon_{1,\alpha,\beta}(\omega)}{2} \right]^{\frac{1}{2}}. \tag{13}$$

The absorption coefficient $A_{\alpha,\beta}(\omega)$ is defined as:

$$A_{\alpha,\beta}(\omega) = \frac{2\kappa_{\alpha,\beta}(\omega)\omega}{c} = \frac{\sqrt{2}\omega}{c} \left[\sqrt{\varepsilon_{1,\alpha,\beta}^2(\omega) + \varepsilon_{2,\alpha,\beta}^2(\omega)} - \varepsilon_{1,\alpha,\beta}(\omega) \right]^{\frac{1}{2}}. \tag{14}$$

where c is the light speed. The reflectivity $R_{\alpha,\beta}(\omega)$ is defined by the refractive index and extinction coefficient by the following expression:

$$R_{\alpha,\beta}(\omega) = \frac{(n_{\alpha,\beta}(\omega) - 1)^2 + \kappa_{\alpha,\beta}^2(\omega)}{(n_{\alpha,\beta}(\omega) + 1)^2 + \kappa_{\alpha,\beta}^2(\omega)}. \tag{15}$$

The energy loss function $L_{\alpha,\beta}(\omega)$ is defined as:

$$L_{\alpha,\beta}(\omega) = \frac{\varepsilon_{2,\alpha,\beta}}{\varepsilon_{1,\alpha,\beta}^2 + \varepsilon_{2,\alpha,\beta}^2}. \tag{16}$$

3.2 Berry Curvature

In solid state physics, the crystal symmetry rules the electronic band structure, as well as the nature of Bloch states. For the crystal with inversion symmetry, the valley magnetic moment and Berry curvature of the Bloch states are zero.[3] Nevertheless, in crystals with inversion asymmetry such as the WS_2/MoS_2 vdWs heterostructure, they are nonzero.[3–5] Moreover, time reversal symmetry requires all Berry-phase related physical quantities to be valley-contrasting. The presence of an external magnetic field or an exchange field exerted, for instance by magnetic substrates, however, breaks time reversal symmetry the valley magnetic moment gives rise to different energy shift in the two valleys. This provides the remarkable possibility of tuning valley splitting exploring different external mechanisms. To gain further insight into the valley dynamics of the interlayer exciton, let us first explore the spin (and valley) Berry curvature $m_n(\mathbf{k})$

and the magnetic moment $\Omega_n(\mathbf{k})$. These two quantities can be calculated by the following general expressions[3,5,6].

$$\Omega_n(\mathbf{k}) = i\langle \nabla_\mathbf{k} \mathbf{u_n} | \times | \nabla_\mathbf{k} \mathbf{u_n} \rangle$$

$$m_n(\mathbf{k}) = -i\frac{e}{\hbar}\langle \nabla_\mathbf{k} \mathbf{u_n} | \times (\mathbf{H_{k\cdot p}} - \mathbf{E_n}) | \nabla_\mathbf{k} \mathbf{u_n} \rangle, \tag{17}$$

where $|u_n\rangle$ and E_n are the n-th Bloch state and its corresponding energy of the effective Hamiltonian $H_{k\cdot p}$, and k is components of wavevector $\mathbf{k}$. In the framework of k·p model, we have performed numerical calculations to obtain the low energy band structure. Once the energy bands and the wavefunctions are obtained, the $\Omega_n(\mathbf{k})$ and $m_n(\mathbf{k})$ of the WS$_2$/MoS$_2$ vdWs heterostructure are calculated using Eq. 17.[7]

In this code, one can obtain the total Berry curvature (semiconductors only) either along certain $\mathbf{k}$-path (KPATH_FILE), using the flag BERRY= T, or the whole Brillouin zone, using the flag BERRY_BZ= T. Total Berry curvature $\Omega_{\alpha,\beta}(\mathbf{k})$ are written by the following expression:

$$\Omega_{\alpha,\beta}(\mathbf{k}) = -2Im\sum_{v,c}\frac{\langle c,\mathbf{k}|P_\alpha|v,\mathbf{k}\rangle\langle v,\mathbf{k}|P_\beta|c,\mathbf{k}\rangle}{(E_{c,\mathbf{k}} - E_{v,\mathbf{k}})^2} \ . \tag{18}$$

The code only outputs the non-zero $\Omega_{\alpha,\beta}(\mathbf{k})$ components: $\Omega_{x,y}(\mathbf{k})$, $\Omega_{x,z}(\mathbf{k})$ and $\Omega_{y,z}(\mathbf{k})$. More details of Berry curvature calculation in the scope of maximally localized Wannier functions, can be found in Wang's work.[8]

3.3 Bethe–Salpeter Formalism

The excitonic states are obtained through the solution of the two-particle problem via the Bethe–Salpeter equation (BSE).[9,10] The excitonic Hamiltonian, H_{exc}, is composed by the electron, H_e, and hole, H_h, single particle Hamiltonians plus Coulomb interaction potential, V_{eh}, which binds the electron-hole pairs, i.e.,

$$H_{exc} = H_e + H_h + V_{eh} \ . \tag{19}$$

The excitonic states with momentum center of mass $\mathbf{Q}$ can be expanded in terms of the

product of electron and hole pairs wave functions, as follows,

$$\Psi_{ex}^{n}(\mathbf{Q}) = \sum_{c,v,\mathbf{k}} A_{c,v,\mathbf{k},\mathbf{Q}}^{n} \left(|c,\mathbf{k}+\mathbf{Q}\rangle \otimes |v,\mathbf{k}\rangle \right), \tag{20}$$

where the index c e v corresponds to the conduction and valence bands states, with momentum $\mathbf{k}+\mathbf{Q}$ and $\mathbf{k}$, respectively. The problem of excitons eigenvalues, can be transformed into BSE,[11] using the expansion of Equation 20, it reads,

$$(E_{c,\mathbf{k}+\mathbf{Q}} - E_{v,\mathbf{k}}) A_{c,v,\mathbf{k},\mathbf{Q}}^{n} + \frac{1}{N_k} \sum_{\mathbf{k}',v',c'} W_{(\mathbf{k},v,c),(\mathbf{k}',v',c'),\mathbf{Q}} A_{c',v',\mathbf{k}',\mathbf{Q}}^{n} = E_{\mathbf{Q}}^{n} A_{c,v,\mathbf{k},\mathbf{Q}}^{n}, \tag{21}$$

where $E_{\mathbf{Q}}^{n}$ are the energy of n-th excitonic state with momentum $\mathbf{Q}$, $A_{c,v,\mathbf{k},\mathbf{Q}}^{n}$ are the exciton wave function (eigenvector), which are obtained by solving Equation 21. $E_{c,\mathbf{k}+\mathbf{Q}} - E_{v,\mathbf{k}}$ are the single-particle energy difference between a conduction band state c with momentum $\mathbf{k}+\mathbf{Q}$ and a valence band state v with momentum $\mathbf{k}$, and $W_{(\mathbf{k},v,c),(\mathbf{k}',v',c'),\mathbf{Q}}$ are the many-body Coulomb interaction matrix element, which can be divided into two parts, direct interaction, W^{d}, and exchange interaction, W^{x}, respectively, i.e.,

$$W_{(\mathbf{k},v,c),(\mathbf{k}',v',c'),\mathbf{Q}} = W_{(\mathbf{k},v,c),(\mathbf{k}',v',c'),\mathbf{Q}}^{d} + W_{(\mathbf{k},v,c),(\mathbf{k}',v',c'),\mathbf{Q}}^{x}. \tag{22}$$

Since the Coulomb potential varies slightly inside unit cell in comparison with Bloch functions, we can approximate the orbital character of Coulomb term in the following way:

$$W_{(\mathbf{k},v,c),(\mathbf{k}',v',c'),\mathbf{Q}}^{d} = V(\mathbf{k}-\mathbf{k}') \langle c,\mathbf{k}+\mathbf{Q}|c',\mathbf{k}'+\mathbf{Q}\rangle \langle v',\mathbf{k}'|v,\mathbf{k}\rangle \tag{23}$$

and

$$W_{(\mathbf{k},v,c),(\mathbf{k}',v',c'),\mathbf{Q}}^{x} = -V(\mathbf{Q}) \langle c,\mathbf{k}+\mathbf{Q}|v,\mathbf{k}\rangle \langle v',\mathbf{k}'|c',\mathbf{k}'+\mathbf{Q}\rangle, \tag{24}$$

where, N_k is the number of $\mathbf{k}$-points in the BZ.

In BSE formalism, the real and imaginary parts of the frequency dependent dielectric tensor $\varepsilon_{1,\alpha,\beta}^{BSE}(\omega)$ and $\varepsilon_{2,\alpha,\beta}^{BSE}(\omega)$ are obtained from the following expressions:

$$\varepsilon_{1,\alpha,\beta}^{BSE}(\omega) = \delta_{\alpha,\beta} + \frac{e^2 S_p}{\varepsilon_0 \Omega N_{\mathbf{k}}} \sum_n F_{\alpha,\beta}^{n,BSE} \frac{E_0^n - \hbar\omega}{\left(\hbar\omega - E_0^n\right)^2 + \eta^2} \, , \tag{25}$$

$$\varepsilon_{2,\alpha,\beta}^{BSE}(\omega) = \frac{e^2 S_p}{\varepsilon_0 \Omega N_{\mathbf{k}}} \sum_n F_{\alpha,\beta}^{n,BSE} \frac{\eta}{\left(\hbar\omega - E_0^n\right)^2 + \eta^2} \, , \tag{26}$$

where E_0^n is the n-th direct $(\mathbf{Q} = 0)$ excitonic state energy, $F_{\alpha,\beta}^{n,BSE}$ is the excitonic modulated oscillator force, given by,

$$F_{\alpha,\beta}^{n,BSE} = \left(\sum_{c,v,\mathbf{k}} \frac{A_{c,v,\mathbf{k},0}^n \langle c,\mathbf{k}|P_\alpha|v,\mathbf{k}\rangle}{(E_{c,\mathbf{k}} - E_{v,\mathbf{k}} + i\eta_1)} \right) \left(\sum_{c',v',\mathbf{k}'} \frac{A_{c',v',\mathbf{k}',0}^{n*} \langle v',\mathbf{k}'|P_\beta|c',\mathbf{k}'\rangle}{(E_{c',\mathbf{k}'} - E_{v',\mathbf{k}'} - i\eta_1)} \right) \, . \tag{27}$$

3.4 Finite temperature BSE approach

Our code also allows one to calculate the exciton energy levels, dielectric functions and other optical properties at a finite temperature for the excitons with $\mathbf{Q} = 0$ by the flags BSET= T, and BSET_BND= T to calculate exciton band structure. These flags cannot be combined with their counterparts without thermal effects BSE= T and BSE_BND= T, respectively. To incoporate the temperature effects, we have to modify BSE as follows[12–14]

$$\left(\Xi_{c,\mathbf{k}+\mathbf{Q}} - E_{v,\mathbf{k}}\right) A_{c,v,\mathbf{k},\mathbf{Q}}^n + \frac{\left(f(E_{v,\mathbf{k}}) - f(\Xi_{c,\mathbf{k}+\mathbf{Q}})\right)}{N_k} \sum_{\mathbf{k}',v',c'} W_{(\mathbf{k},v,c),(\mathbf{k}',v',c'),\mathbf{Q}} \, A_{c',v',\mathbf{k}',\mathbf{Q}}^n = E_{\mathbf{Q}}^n A_{c,v,\mathbf{k},\mathbf{Q}}^n \, , \tag{28}$$

where $f(E)$ is the Fermi-Dirac distribution, and $\Xi_{c,\mathbf{k}+\mathbf{Q}}$ is the conduction band energy with a correction of temperature effects, defined as :

$$\Xi_{c,\mathbf{k}+\mathbf{Q}} = E_{c,\mathbf{k}+\mathbf{Q}} - \Delta(\alpha_B, \Theta, T) \, , \tag{29}$$

where T is the temperature in K, given by the flag `TEMP`, α_B and Θ are empirical parameters to be fitted to experimental data, given by the flags `ST` and `PHAVG`, respectively, and the analytical expression of the correction $\Delta(\alpha_B, \Theta, T)$ depends on the the approximations made in the calculation. Usually, the following three formulations have been widely used in the literature. The first one is the frozen atom approximation in which we assume $\Delta(\alpha_B, \Theta, T) = 0$, given by the flag `TA= FA`. The second one is Bose-Einstein approximation,[15] given by the flag `TA= BE`, where

$$\Delta(a_B, \Theta, T) = \frac{2a_B}{e^{\Theta/T} - 1} \; , \tag{30}$$

where α_B represents the strength of electron-phonon interactions in eV and Θ is the average phonon temperature in K. The third one is given by the flag `TA= VE`, in which the correction term is described by,[16]

$$\Delta(\alpha_B, \Theta, T) = \alpha_B \Theta \left[coth \left(\frac{\alpha_B}{2k_b T} \right) - 1 \right] \; , \tag{31}$$

where Θ is a dimensionless coupling constant and α_B is an average of phonon energy in eV.

These temperature effects also correct the expressions for the oscillator force $F_{\alpha,\beta}^{c,v,\mathbf{k}}$ and excitonic modulated oscillator force $F_{\alpha,\beta}^{n,BSE}$ by

$$F_{\alpha,\beta}^{c,v,\mathbf{k}} = \frac{\langle c,\mathbf{k}|P_\alpha|v,\mathbf{k}\rangle \langle v,\mathbf{k}|P_\beta|c,\mathbf{k}\rangle}{(\Xi_{c,\mathbf{k}} - E_{v,\mathbf{k}} - i\eta_1)(\Xi_{c,\mathbf{k}} - E_{v,\mathbf{k}} + i\eta_1)} \left(f(E_{v,\mathbf{k}}) - f(\Xi_{c,\mathbf{k}}) \right) \; , \tag{32}$$

$$F_{\alpha,\beta}^{n,BSE} = \left(\sum_{c,v,\mathbf{k}} \frac{A_{c,v,\mathbf{k},0}^n \langle c,\mathbf{k}|P_\alpha|v,\mathbf{k}\rangle}{(\Xi_{c,\mathbf{k}} - E_{v,\mathbf{k}} + i\eta_1)} \right) \left(\sum_{c',v',\mathbf{k}'} \frac{A_{c',v',\mathbf{k}',0}^{n*} \langle v',\mathbf{k}'|P_\beta|c',\mathbf{k}'\rangle}{(\Xi_{c',\mathbf{k}'} - E_{v',\mathbf{k}'} - i\eta_1)} \right) \left(f(E_{v',\mathbf{k}'}) - f(\Xi_{c',\mathbf{k}'}) \right) \; . \tag{33}$$

3.5 Coulomb Potentials

Our code posses several options for the Coulomb interaction $V_e h$ (reciprocal space) in the BSE formalism. In this section we'll briefly discuss each of them. To avoid divergence in these

potentials, a tolerance parameter $\mathbf{Q}_{tol}$ was introduced in our implementation, its value given by the flag `KTOL`.

3.5.1 Bare Coulomb Potential (V3D)

This is the traditional Coulomb Potential in reciprocal space, being identified by the input flag `COULOMB_POT= V3D`, and described by the following expression

$$V(\mathbf{Q}) = -\frac{e^2}{2V_{uc}\varepsilon_0\mathbf{Q}^2} \, , \tag{34}$$

where V_{uc} is the unit cell volume. To avoid the divergence at $\mathbf{Q} \to 0$, we define

$$V(|\mathbf{Q}| < \mathbf{Q_{tol}}) = 0 \, . \tag{35}$$

3.5.2 Screened Coulomb Potential (V3DL)

This is a variation of the Bare Coulomb potential considering a dielectric screening, which could be used to control exciton binding energy and adjust the results with experimental measurements.It's identified by the flag `COULOMB_POT= V3DL` in main input file, and described as the following

$$V(\mathbf{Q}) = -\frac{e^2}{2V_{uc}\varepsilon_0\varepsilon_d\mathbf{Q}^2} \, , \tag{36}$$

where ε_d is parameter given in the main input file by the flag `EDIEL`.

3.5.3 2D Keldysh Potential(V2DK)

A Keldysh type Coulomb potential normally be used to properly describe the 2D Coulomb interaction.[17] It's selected by the flag `COULOMB_POT= V2DK` in main input file, with the following equation

$$V(\mathbf{Q}) = -\frac{e^2}{2A_{uc}\varepsilon_0\varepsilon_d|\mathbf{Q}|(1+r_0|\mathbf{Q}|)} \, . \tag{37}$$

with the objective to avoid Coulomb potential singularity, we make the following approximation for $|\mathbf{Q}| \leq \mathbf{Q}_{tol}$,

$$V(|\mathbf{Q}| \leq \mathbf{Q}_{tol}) = \frac{-e^2 a N_k}{4\pi A_{uc}\varepsilon_0 \varepsilon_d} \left[\alpha_1 + \alpha_2 \Delta + \alpha_3 \Delta^2\right], \tag{38}$$

where $\Delta = 2\pi r_0 / a N_k$, and $\alpha_1 = 1.76$, $\alpha_2 = 1$, and $\alpha_3 = 0.$[9,17] N_k is the number of **k**-points used in **k**-mesh, A_{uc} is the unit cell area and a is the average of the first and second lattice vectors size. The Coulomb potential screening length r_0 is given by the expression:

$$r_0 = l_c \frac{(\varepsilon_2 - 1)}{(\varepsilon_1 + \varepsilon_3)}, \tag{39}$$

and the effective dielectric constant ε_d is given by:

$$\varepsilon_d = \frac{\varepsilon_1 + \varepsilon_3}{2} \tag{40}$$

where l_c is a free parameter, given by the flag LC, that corresponds to the third lattice vector size or the distance between two neighbor layers of the 2D systems, ε_2 are in plane macroscopic effective dielectric constant, given in the main input file by the flag EDIEL, ε_1 and ε_3 corresponds to the dielectric constants of the substrate above and bellow, given by the flags EDIEL_T and EDIEL_B respectively.

3.5.4 2D Rytova–Keldysh Potential (V2DRK)

2D Rytova–Keldysh Potential is another version of a Keldysh type Coulomb potential used for 2D systems.[18] It's selected by the flag COULOMB_POT= V2DRK in main input file, being described,

$$V(\mathbf{Q}) = -\frac{e^2}{2A_{uc}\varepsilon_0|\mathbf{Q}|F(\mathbf{Q})} e^{-w_0|\mathbf{Q}|}, \tag{41}$$

where

$$F(\mathbf{Q}) = \frac{\left[1 - \left(p_b\, p_t\, e^{-2|\mathbf{Q}|\eta l_c}\right)\right]\kappa}{\left[1 - \left(p_t e^{-\eta|\mathbf{Q}|l_c}\right)\right]\left[1 - \left(p_b e^{-\eta|\mathbf{Q}|l_c}\right)\right]} + r_0|\mathbf{Q}|e^{-w_0|\mathbf{Q}|} \tag{42}$$

and

$$p_b = \frac{\varepsilon_b - \kappa}{\varepsilon_b + \kappa} ,$$
$$p_t = \frac{\varepsilon_t - \kappa}{\varepsilon_t + \kappa} ,$$
$$\kappa = \sqrt{\varepsilon_2 \varepsilon_z} ,$$
$$\eta = \sqrt{\frac{\varepsilon_2}{\varepsilon_z}} , \tag{43}$$

where A_{uc} is the area of crystal unit cell, w_0 and r_0 are free parameters given by the flags `W_COUL` and `R_0` respectively. ε_2 is the in plane effective dielectric constant of the crystal, given in the main input file by the flag `EDIEL`, ε_z is the out of plane effective dielectric constant of the crystal, given by the flag `EDIEL_Z`, ε_b is the dielectric constant of the environment bellow the 2D system, given by the flag `EDIEL_B`, ε_t is the dielectric constant of the environment above the 2D system, given by the flag `EDIEL_T`. l_c refers to the crystal thickness (in Å), given by the flag `LC`.

To avoid the divergence at $\mathbf{Q} \to 0$, we consider the following

$$V(|\mathbf{Q}| < \mathbf{Q_{tol}}) = 0 . \tag{44}$$

3.5.5   2D Ohno Potential (V2DOH)

Ohno Coulomb potential for 2D systems,[19] being selected by the flag `COULOMB_POT= V2DOH` in main input file. It is given by the following expression:

$$V(\mathbf{Q}) = -\frac{e^2}{2A_{uc}\varepsilon_0\varepsilon_d|\mathbf{Q}|} e^{-w_0|\mathbf{Q}|} , \tag{45}$$

where A_{uc} is the unit cell area, ε_d is an effective dielectric constant parameter, given by the flag `EDIEL`, w_0 is a free parameter given by the flag `W_COUL`.

To avoid the divergence at $\mathbf{Q} \to 0$, we define

$$V(|\mathbf{Q}| < \mathbf{Q_{tol}}) = 0 . \tag{46}$$

3.5.6 2D truncated Coulomb Potential (V2DT)

A Coulomb potential truncated for 2D systems, proposed by Rozzi *et. al.*[20] being selected by the flag COULOMB_POT= V2DT in main input file. This potential has the following expression:

$$V(\mathbf{Q}) = -\frac{e^2}{2V_{uc}\varepsilon_0 \mathbf{Q}^2}\left[1 - e^{-C_2}\left(C_1 \sin(C_3) - \cos(C_3)\right)\right], \qquad (47)$$

where V_{uc} is volume of the unit cell and $\mathbf{r}_3$ is the size of the third lattice vector (real space). C_1, C_2 and C_3 are defined as,

$$C_1 = \frac{|Q_z|}{\sqrt{Q_x^2 + Q_y^2}},$$
$$C_2 = \frac{\mathbf{r}_3}{2}\sqrt{Q_x^2 + Q_y^2},$$
$$C_3 = \frac{\mathbf{r}_3}{2}|Q_z|. \qquad (48)$$

If $\sqrt{Q_x^2 + Q_y^2} < |\mathbf{Q}_{tol}|$ and $|Q_z| \geq |\mathbf{Q}_{tol}|$, then the Coulomb potential is described by,

$$V(\mathbf{Q}) = -\frac{e^2}{2V_{uc}\varepsilon_0 \mathbf{Q}^2}\left[1 - \cos(0.5|Q_z|\mathbf{r}_3) - (0.5|Q_z|\mathbf{r}_3)\sin(0.5|Q_z|\mathbf{r}_3)\right]. \qquad (49)$$

Else if $\sqrt{Q_x^2 + Q_y^2} < |\mathbf{Q}_{tol}|$ and $|Q_z| < |\mathbf{Q}_{tol}|$, then Coulomb potential becomes,

$$V(\mathbf{Q}) = -\frac{e^2}{2V_{uc}\varepsilon_0}\left(\frac{\mathbf{r}_3^2}{8}\right), \qquad (50)$$

3.5.7 2D truncated simplified Coulomb Potential (V2DT2)

A variation for the truncated Coulomb potential for 2D systems proposed by IsmailBeigi *et. al.*[21] being selected by the flag COULOMB_POT= V2DT2 in main input file. It has the following expression:

$$V(\mathbf{Q}) = -\frac{e^2}{2V_{uc}\varepsilon_0 \mathbf{Q}^2}\left[1 - e^{-Q_{xy}Z_c}\cos(Q_z Z_c)\right], \qquad (51)$$

where $Q_{xy} = \sqrt{(Q_x^2 + Q_y^2)}$, V_{uc} is the unit cell volume and Z_c is half of the lattice vector in $\hat{z}$ direction, given by the flag LC.

To avoid the divergence at $\mathbf{Q} \to 0$, we suppose

$$V(|\mathbf{Q}| < \mathbf{Q_{tol}}) = 0 . \tag{52}$$

3.5.8   1D truncated Coulomb Potential (V1DT)

A Coulomb potential truncated for 1D systems, proposed by Rozzi *et. al.*[20] being selected by the flag COULOMB_POT= V1DT in main input file, considering the periodicity in $\hat{x}$ direction. This potential has the following expression:

$$V(\mathbf{Q}) = -\frac{e^2}{2V_{uc}\varepsilon_0\mathbf{Q}^2} [1 + C_1 - C_2] \tag{53}$$

where V_{uc} is the unit cell volume and R, given by the flag LC, is the radius of the cylindrical cutoff in Å, used to obtain this 1D potential, C_1, C_2 and Q_{yz} are defined by the following expressions:

$$C_1 = Q_{yz}RJ_1\left(Q_{yz}R\right)K_0\left(|Q_x|R\right) ,$$
$$C_2 = |Q_x|RJ_0\left(Q_{yz}R\right)K_1\left(|Q_x|R\right) ,$$
$$Q_{yz} = \sqrt{Q_y^2 + Q_z^2} , \tag{54}$$

J and K are the ordinary and modified cylindrical Bessel functions.

If $|Q_x| < Q_{tol}$ and $|Q_{yz}| \geq Q_{tol}$, then the Coulomb potential is described by,

$$V(\mathbf{Q}) = -\frac{e^2}{2V_{uc}\varepsilon_0} \int_0^R rJ_0(Q_{yz}r)ln(r)dr \tag{55}$$

Else if $|Q_x| < Q_{tol}$ and $|Q_{yz}| < Q_{tol}$, the the Coulomb potential becomes,

$$V(\mathbf{Q}) = -\frac{e^2}{2V_{uc}\varepsilon_0} \left(\frac{R^2}{16}\right) [2ln(R) - 1]. \tag{56}$$

3.5.9 0D Potential (V0DT)

An adaption of the Coulomb potential for 0D systems, proposed by Rozzi *et. al.*,[20] being selected by the flag COULOMB_POT= V0DT in main input file. It is described by the following expression:

$$V(\mathbf{Q}) = -\frac{e^2}{2V_{uc}\varepsilon_0\mathbf{Q}^2}\left[1 - \cos(0.5\mathbf{r}_{min}|\mathbf{Q}|)\right] \tag{57}$$

To avoid the divergence at $\mathbf{Q} \to 0$, we consider the following condition

$$V(|\mathbf{Q}| < \mathbf{Q_{tol}}) = -\frac{e^2}{2V_{uc}\varepsilon_0}\left(\frac{\mathbf{r}_{min}^2}{8}\right) . \tag{58}$$

where V_{uc} is the unit cell volume and $\mathbf{r}_{min}$ is the size of the smallest lattice vector (real space).

3.6 Exciton radiative lifetime

In this code the exciton radiative lifetime is calculated directly from the excitonic state oscillator force ($F_{\alpha,\beta}^{n,BSE}$), described in equation 27. Being calculated using the flag BSE= T combined with SPEC= T, where the lifetime is obtained in seconds. This quantity is only calculated for direct excitons.

For 3D systems (SYSDIM= 3D), the lifetime, for the n-th excitonic states, is obtained by,[22]

$$\tau_{3D,\alpha,\beta}^n = \frac{3c^2\hbar^3N_{\mathbf{k}}}{4\chi\left(E_0^n\right)^3 F_{\alpha,\beta}^{n,BSE}} . \tag{59}$$

While for 2D systems (SYSDIM= 2D), a similar expression is given by,[23]

$$\tau_{2D,\alpha,\beta}^n = \frac{\hbar A_{uc}N_{\mathbf{k}}}{8\pi\chi E_0^n F_{\alpha,\beta}^{n,BSE}} . \tag{60}$$

Finally for 1D systems (SYSDIM= 1D), it is described by[22]

$$\tau_{1D,\alpha,\beta}^n = \frac{c\hbar^2\mathbf{r}_1 N_{\mathbf{k}}}{2\pi\chi\left(E_0^n\right)^2 F_{\alpha,\beta}^{n,BSE}} , \tag{61}$$

where c is the light speed, E_0^n is the n-th excitonic state energy, A_{uc} is the 2D crystal unit cell area, $\mathbf{r}_1$ is the 1D unit cell size and χ is the fine structure constant, given by:

$$\chi = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx \frac{1}{137} \, .$$

(62)

3.7 k-mesh generator

The **k**-meshes are generated using the Monkhorst–Pack scheme,[24] where the **k**-points are defined by the following expression:

$$\mathbf{k} = \frac{n_1}{\text{NGX}}\mathbf{b}_1 + \frac{n_2}{\text{NGY}}\mathbf{b}_2 + \frac{n_3}{\text{NGZ}}\mathbf{b}_3 + \mathbf{s}$$

(63)

where NGX, NGY and NGz are the number of grid points along x-, y and z-directions, respectively, $n_1 = 0\ldots,(\text{NGX}-1)$, $n_2 = 0\ldots,(\text{NGY}-1)$, $n_3 = 0\ldots,(\text{NGZ}-1)$, $\mathbf{b}_i$ denote the lattice reciprocal vectors and **s** is the mesh shift vector, where their components are attributed to the flags SHIFT_1, SHIFT_2 and SHIFT_3 respectively.

If the user wouldn't like to specify directly the **k**-mesh size using the flags NGX, NGY and NGZ in the input file, it's possible to define it through the flags MESH_TYPE= RK3D or MESH_TYPE= RK2D, choosing a density of **k**-points defined by the flag RK. The values of NGX, NGY and NGZ, are obtained for the option MESH_TYPE= RK3D by the following expression:

$$NGX = int\left(max\left(1, \text{RK}\frac{|\mathbf{b}_1|}{2\pi} + 0.5\right)\right)$$
$$NGY = int\left(max\left(1, \text{RK}\frac{|\mathbf{b}_2|}{2\pi} + 0.5\right)\right)$$
$$NGZ = int\left(max\left(1, \text{RK}\frac{|\mathbf{b}_3|}{2\pi} + 0.5\right)\right)$$

(64)

for the option MESH_TYPE= RK2D the only difference is that NGZ=1 independent of RK.

3.8 Solar Cell Power Conversion Efficiency

In this code it's available to estimate the power conversion efficiency (PCE), of the studied system, in the scope of Shockley-Queisser Limit (SQ-limit),[25] and spectroscopy limited maximum efficiency (SLME) scheme.[26] This simulation is available by the input flag PCE= T.

Both approximations are based on the principle of detailed balance between absorbed photons and emitted photons. Below, we will summarize the mathematical formalism[27] and the SQ-limit and SLME approximations.

The PCE is defined as the maximum output power density (P_{PV}) from the photovoltaic device divided by the total incoming power density from the solar spectrum, P_{solar}, as follows,

$$\text{PCE} = \frac{P_{PV}}{P_{solar}} , \tag{65}$$

where

$$P_{solar} = \int_0^\infty P(E) dE , \tag{66}$$

and $P(E)$ is the solar energy flux, which is selected by the flag SES, and has the options: AM15G, AM15D and AM0G, which corresponds to the standard solar spectrum for non-concentrated photovoltaic conversion, taking light absorption and scattering in the atmosphere into account.[28] The output power density is described by the product $J(V)V$, as the maximum output power density (P_{PV}) is obtained maximizing the $J - V$ characteristic of an illuminated solar cell :

$$P_{PV} = J(V_{max})V_{max} , \tag{67}$$

where V_{max} is the voltage that results in the maximum output power density. The open circuit voltage V_{oc} is the voltage that minimizes $J(V)$. In this method, the current density, $J(V)$, are described by the following expression:

$$J(V) = J_{sc} - \frac{J_0}{fr} \left(exp \left(\frac{eV}{k_B T} \right) - 1 \right) , \tag{68}$$

where k_B is Boltzmann's constant, e is the elementary charge, fr is the radiative electron-hole

recombination fraction and T is the temperature of the solar cell, defined by the flag `CTEMP`. J_{sc} is the short-circuit current density, also known as the illuminated current or photogenerated current, calculated from the following expression,

$$J_{sc} = e \int_0^\infty a(E) \frac{P(E)}{E} dE \ . \tag{69}$$

$a(E)$ is the absorbance, which is defined as the ratio of power absorbed by the solar device over the power of incident sunlight.

J_0 is the reverse saturation current density, calculated considering the detailed balance principle when in equilibrium conditions, the photon emission rate from radiative recombination is equal to the photon absorption from the surrounding environment. This was done considering our solar cell attached to an ideal heat sink, expecting the cell temperature to be the ambient temperature. Hence, the spectrum of the surrounding environment is that of a black body at cell temperature T,

$$J_0 = e\pi \int_0^\infty a(E) \Phi_{bb}(E) dE \ , \tag{70}$$

where,

$$\Phi_{bb}(E) = \frac{2E^2}{h^3 v_c^2} \left(e^{\frac{E}{k_B T}} - 1 \right)^{-1} \ , \tag{71}$$

and h is Planck's constant and v_c is the speed of light. Complementary we can also calculate the Fill-Factor (FF) of our solar device, by the expression:

$$FF = \frac{V_{max} J(V_{max})}{V_{oc} J_{sc}} \ . \tag{72}$$

3.8.1 Shockley–Queisser Limit

In the SQ-limit approximation, we consider the absorbance, $a(E)$, as a Heaviside step function, where all photons with energy higher or equal to the energy bandgap, E_g, are absorbed, i.e., $a(E) = 1$ for $E \geq E_g$, and $a(E) = 0$ for $E < E_g$. Furthermore, this approximation assumes $fr = 1$, i.e., the radiative recombination process is the only recombination process for all systems, neglecting the non-radiative recombinations (e.g., Auger recombination) due to indirect bandgap.[29,30]

3.8.2 Spectroscopy Limited Maximum Efficiency

In contrast with the SQ-limit approach, the SLME approximation requires the total absorption coefficient,

$$A(\omega) = A_{x,x}(\omega) + A_{y,y}(\omega) + A_{z,z}(\omega) , \tag{73}$$

material thickness, Δ, and the bandgaps. Its also considers the non-radiative recombination in the solar cell by modeling the fraction of radiative recombination, fr, using a Boltzmann factor,[26]

$$fr = e^{-\frac{\delta}{k_B T}} \tag{74}$$

for calculations in the scope of IPA (without excitons), we can define $\delta = E_{op} - E_g$, where E_{op} is the optical bandgap, given by the flag `EGD` and E_g is the fundamental energy bandgap, given by the flag `EG`. In the scope of BSE (with excitonic effects), we can define $\delta = Ex_{br} - Ex_{gs}$, where Ex_{br} is the exciton bright ground state (optical bandgap considering excitonic effects), given by the flag `EBGS`, while Ex_{gs} is the exciton ground state, given by the flag `EGS`. The absorbance, $a(E)$, is obtained considering the solar cell with the same conditions of SQ-Limit described previously, given by the following expression,[26,31]

$$a(E) = 1 - e^{-2 A(\omega) \Delta} , \tag{75}$$

where $E = \hbar\omega$, and Δ is the material thickness, in this code we calculate the PCE, in the scope of SLME method from $\Delta = 0$ until $\Delta = \Delta_{max}$, being Δ_{max} defined by the flag `THMAX`.

4 Input files

4.1 Main input

The execution of this code need a main input file, where the names of the other input files are contained in this file (The main input file contains the names of the other input files are contained in this file). An example of this main input file are (is) shown in Figure S1. In this file the order of the flags are (is) not important.

```
NTHREADS= 10
SYSDIM= "2D"

PARAMS_FILE= "tb_hr.dat"
KPATH_FILE= "kpoints.dat"
KPATH_BSE= "kpoints-bse.dat"
OUTPUT= "./out/"
CALC_DATA= "./out/"

COULOMB_POT= "V2DK"
EDIEL_T=   1.0000
EDIEL_B=   4.0000
LC= 24.0

MESH_TYPE= "RK2D"

 RK= 120.0

 NBANDSC=  2
 NBANDSV=  2

 EXC_WF_I= 1
 EXC_WF_F= 10

 BSE_BND= T
 BSE_WF= T
 BSE= T

 BANDS= T
 DOS= F
```

Figure S1: Example of the main input file.

All flag options used in the main input file are listened bellow. In this main input file when writing each flag (flags) it's important to do this in this way: `FLAG= Value`, if written in other way (i.e `FLAG = Value`) (otherwise, e.g., `FLAG = Value`) the flag will be ignored by the code.

4.1.1 `integer :: NTHREADS`

Default value :: 1

Description: Number of threads used to run the code in parallel with OpenMP.

4.1.2 `character(len=2) :: SYSDIM`

Default value :: 3D

Available values :: 3D, 2D, 1D

Description: Used to define the dimensions of your system, it's used to select the correct expression to calculate exciton lifetime, showed in section 3.6. (It is used to define the dimension

of your system so that a proper expression of Coulomb interaction is chosen to calculate exciton lifetime, see section 3.6)

4.1.3 `character(len=1) ::  DFT`

Default value :: V

Available values :: V or O

Description: Uses (Chose) V if obtained the wannierization from VASP package, using the patch for MLWF, available in: `https://github.com/Chengcheng-Xiao/VASP2WAN90_v2_fix`, or O if another DFT code is used (otherwise, for other DFT packages, select "O"). It's used to performs (perform) SpinDOS and band structure calculations with average values of S_z operator.

4.1.4 `character(len=2) ::  TA`

Default value :: FA

Available values :: FA, BE, VE

Description: Used to define the bandgap correction due to temperature effects, see section 3.4 more details.

4.1.5 `character(len=70) ::  PARAMS_FILE`

Mandatory flag to run the code

Description: Localization of the TB parameters file.

4.1.6 `character(len=70) ::  OUTPUT`

Default value :: ./

Description: Folder to put the output files generated by the code (Folder where the output files generated by the code are stored).

4.1.7 `character(len=70) ::  CALC_DATA`

Default value :: ./

Description: Folder to put the output log files generated by the code. (Folder which contains the output log files generated by the code.)

4.1.8 `character(len=70) ::  KPATH_FILE`

Default value :: non declared file

Description: Localization for the file with the **k**-path (Directory which contains the file of **k**-path) used for electronic structure and berry curvature calculations. More information in section. 4.4

4.1.9 `character(len=70) ::  KPATH_BSE`

Default value :: non declared file

Description: Localization for the file with the **k**-path (Directory which contains the file of **k**-path) used for BSE structure calculations. Same format of `KPATH_FILE`. (The same format as `KPATH_FILE` is used). More information (can be found) in section. 4.4

4.1.10 `character(len=70) ::  ORB_W`

Default value :: non declared file

Description: Localization of the file with the selected orbitals to make projected DOS and band structure (Directory which contains the file where the selected orbitals are stored to make projected DOS and band structure calculation) using orbital contribution color code. More information (can be found) in section. 4.3

4.1.11 `logical ::  BANDS`

Default value :: F

Description: `BANDS= T` run electronic band structure calculation.

4.1.12 `logical :: DOS`

Default value :: F

Description: `DOS= T` run electronic density of states calculation, if the parameters are obtained from spin-polarized or SOC DFT calculations, also generate SpinDOS. If `ORB_W` file was declared, calculates also PDOS with the selected orbital contribution. (run the calculation of electronic density of states. If the parameters are obtained from spin-polarized or SOC DFT calculations, it gives rise to SpinDOS. In addition, if `ORB_W` file was declared, it can also offer PDOS with the selected orbital contribution.)

4.1.13 `logical :: BSE`

Default value :: F

Description: `BSE= T` run BSE calculation. Gives only direct exciton energies and their oscillator force for each state, using the selected conduction and valence states. Also calculates oscillator force for each direct optical transition, using the selected conduction and valence states. (run BSE calculation. It provides direct exciton energies and oscillator strength of optical transition between conduction and valence bands.)

4.1.14 `logical :: BSET`

Default value :: F

Description: `BSET= T` run BSE calculation with temperature effects, more details in section 3.4. Gives only direct exciton energies and their oscillator force for each state, using the selected conduction and valence states. Also calculates oscillator force for each direct optical transition, using the selected conduction and valence states. (run finite temperature BSE calculation, more detailed information can be found in section 3.4. It provides direct exciton energies and oscillator strength of optical transition between conduction and valence bands at finite temperature.)

4.1.15 `logical :: BSE_BND`

Default value :: F

Description: `BSE_BND= T` run BSE excitonic band structure calculation. Gives indirect exciton

energies, using the selected conduction and valence states. (run BSE excitonic band structure calculation. It provides not only direct, but also indirect exciton energies associated with certain conduction and valence bands.)

4.1.16 `logical :: BSET_BND`

Default value :: F

Description: `BSET_BND= T` run BSE excitonic band structure calculation, with temperature effects, more details in section 3.4. Gives indirect exciton energies, using the selected conduction and valence states. (run finite temperature BSE excitonic band structure calculation. More information can be found in section 3.4 It provides not only direct, but also indirect exciton energies associated with certain conduction and valence bands, at finite temperature.)

4.1.17 `logical :: DIEL`

Default value :: F

Description: `DIEL= T` calculates oscillator force for each direct optical transition, using the selected conduction and valence states. (Calculate oscillator strength of direct optical transition between conduction and valence bands.)

4.1.18 `logical :: OPT_BZ`

Default value :: F

Description: `OPT_BZ= T` calculates oscillator force per **k**-point, using the selected conduction and valence states. (Calculate oscillator strength of direct optical transition between conduction and valence bands for a chosen **k**-point.)

4.1.19 `logical :: SPEC`

Default value :: F

Description: `SPEC= T` calculates dielectric function (real and imaginary parts), absorption coefficient, extinction coefficient, refractive index and reflectibility with (`BSE= T` or `BSET= T`) or without excitonic effects (`DIEL= T`). Also calculates exciton lifetimes. This flag only works

combined with `BSE= T`, `BSET= T` or `DIEL= T`. (Calculate dielectric function (both real and imaginary parts), absorption coefficient, extinction coefficient, refractive index, reflectibility and energy loss function either with excitonic effect at zero temperature (`BSE= T` or finite temperature `BSET= T`) or without excitonic effects (`DIEL= T`). In additon, it also provides exciton lifetimes. This flag only works combining with either `BSE= T`, or `BSET= T` or `DIEL= T`.)

4.1.20 `logical ::  RNMD`

Default value :: T

Description: `RNMD= T` makes a renormalization of the imaginary component of dielectric function.

4.1.21 `logical ::  BERRY_BZ`

Default value :: F

Description: `BERRY_BZ= T` calculates total Berry curvature (semiconductors only) in the entire Brillouin Zone. (`BERRY_BZ= T` calculates total Berry curvature of semiconductors in the entire Brillouin Zone.)

4.1.22 `logical ::  BERRY`

Default value :: F

Description: `BERRY= T` calculates total Berry curvature (semiconductors only) in a selected **k**-path given by the `KPATH_FILE`. (`BERRY= T` calculates total Berry curvature of semiconductors in a selected **k**-path defined by the `KPATH_FILE`.

4.1.23 `logical ::  PP_ONLY`

Default value :: F

Description: `PP_ONLY= T` + `SPEC= T` + `BSE= T` (or `BSET= T`) and/or `DIEL= T`, calculates dielectric function (real and imaginary parts), absorption coefficient, extinction coefficient, refractive index, reflectibility and energy loss function with (`BSE= T`) and/or without excitonic

effects (DIEL= T), and exciton lifetimes, If BSE= T (BSET= T) and/or DIEL= T, was calculated on previous run using SPEC= F . (PP_ONLY= T + SPEC= T + BSE= T (or BSET= T) and/or DIEL= T calculate dielectric function (both real and imaginary parts), absorption coefficient, extinction coefficient, refractive index and reflectibility either with excitonic effect at zero temperature (BSE= T or finite temperature BSET= T) or without excitonic effects (DIEL= T). In additon, it also provides exciton lifetimes. This flag only works combining with either BSE= T, or BSET= T or DIEL= T.

4.1.24 `logical ::  BSE_WF`

Default value :: F

Description: BSE_WF= T returns excitonic wave function output file, from BSE= T (BSET= T) and/or BSE_BND= T (BSET_BND= T) calculations, from the excitonic states defined in the interval EXC_WF_I to EXC_WF_F variables. (BSE_WF= T produces output file of excitonic wave functions for the excitonic states lying in the interval of EXC_WF_I to EXC_WF_F, based on BSE= T (BSET= T) and/or BSE_BND= T (BSET_BND= T) calculations.)

4.1.25 `logical ::  TMCOEF`

Default value :: F

Description: TMCOEF= T generates transition matrix elements (oscillator force) for the optical transitions for each **k**-point, using the selected conduction and valence states. (TMCOEF= T generates transition matrix elements (oscillator strength) of optical transition between certain conduction and valence bands for each **k**-point.)

4.1.26 `logical ::  DTDIAG`

Default value :: F

Description: DTDIAG= T calculate the xy, xz and yz components of dielectric functions from BSE= T (BSET= T) calculation, if DTDIAG= F these components are set to 0 .(DTDIAG= T calculate the xy, xz and yz components of dielectric functions, based on BSE= T (BSET= T) outputs. If DTDIAG= F, they are set to 0 .)

4.1.27 `logical :: CPOL`

Default value :: F

Description: `CPOL= T` calculates the dielectric functions considering the circular polarization, σ_+(sp) and σ_-(sm), from `BSE= T` (`BSET= T`) calculation, if `CPOL= F` these components are set to 0 .(`CPOL= T` calculates the dielectric functions for the circularly polarized excitation light with either σ_+(sp) or σ_-(sm), based on `BSE= T` (`BSET= T`) calculation. If `CPOL= F`, they are are set to 0 .

4.1.28 `logical :: PCE`

Default value :: F

Description: `PCE= T` calculates the power conversion efficiency, for solar cells with the correspondent crystal of `PARAMS_FILE`. For this calculation it is necessary to calculate first the absorption spectrum with or/and without excitonic effects. It's also necessary to informs the selected solar emission spectrum (`SES`), solar cell temperature (`CTEMP`), maximum cell thickness (`THMAX`), fundamental bandgap (`EG`), direct bandgap (`EGD`), exciton ground state energy (`EGS`) and exciton bright ground state energy (`EBGS`). More details in section 3.8. (Description: `PCE= T` calculates the power conversion efficiency for solar cells with the corresponding crystal parameter file of `PARAMS_FILE`. Before performing this calculation, it prerequires to calculate the absorption spectrum with or/and without excitonic effects. It's also required to inform the selected solar emission spectrum (`SES`), solar cell temperature (`CTEMP`), the maximum cell thickness (`THMAX`), the fundamental bandgap (`EG`), direct bandgap (`EGD`), exciton ground state energy (`EGS`) and the ground state energy (`EBGS`) of bright exciton. More informations can be found in section 3.8.)

4.1.29 `integer :: NGX`

Default value :: 1

Description: Sets the number of grid points in the **k**-mesh grid along the first reciprocal lattice vector. More information in section 3.7. (Setting the number of grid points in the **k**-mesh grid along the first reciprocal lattice vector. More information can be found in section 3.7.)

4.1.30 `integer :: NGY`

Default value :: 1

Description: Sets the number of grid points in the **k**-mesh grid along the second reciprocal lattice vector. More information can be found in section 3.7.

4.1.31 `integer :: NGZ`

Default value :: 1

Description: Sets the number of grid points in the **k**-mesh grid along the third reciprocal lattice vector. More information can be found in section 3.7.

4.1.32 `real(kind=dp) :: SHIFT_1`

Default value :: 0.0

Description: First component of the **k**-mesh shift first coordinate, direct units. More information can be found in section 3.7.

4.1.33 `real(kind=dp) :: SHIFT_2`

Default value :: 0.0

Description: Second component of the **k**-mesh shift first coordinate, direct units. More information can be found in section 3.7.

4.1.34 `real(kind=dp) :: SHIFT_3`

Default value :: 0.0

Description: Third component of the **k**-mesh shift first coordinate, direct units. More information can be found in section 3.7.

4.1.35 `character(len=70) :: MESH_TYPE`

Default value :: MKH

Available values :: MKH, RK3D or RK2D

Description: If `MESH_TYPE=` MKH, then generates **k**-mesh with the input variables `NGX`, `NGY`,

NGZ. Otherwise, it creates an Automatic **K**-mesh for 3D or 2D systems, defining NGX, NGY, NGZ for a certain density of **k**-points, given by the flag RK. More information can be found in section 3.7.

4.1.36 `real(kind=dp) :: RK`

Default value :: 0.0

Description: Density of **k**-points used for automatic **k**-mesh generator. More information can be found in section 3.7.

4.1.37 `integer :: NEDOS`

Default value :: 6001

Description: Number of points used in the electronic energy interval in DOS= T calculation.

4.1.38 `real(kind=dp) :: SIGMA`

Default value :: 0.08

Description: Gaussian smearing parameter used in DOS= T calculation.

4.1.39 `integer :: NBANDSC`

Default value :: 1

Description: Number of conduction bands above Fermi level is used for the calculation of optical and excitonic properties.

4.1.40 `integer :: NBANDSV`

Default value :: 1

Description: Number of valence bands, counted from Fermi level, used for the calculation of optical and excitonic properties.

4.1.41 `real(kind=dp) :: ENSPECI`

Default value :: 0.0

Description: Lower limit of photon energy in the calculation of dielectric function and other optical properties.

4.1.42 `real(kind=dp) :: ENSPECF`

Default value :: 3.0

Description: Upper limit of photon energy in the calculation of dielectric function and other optical properties.

4.1.43 `integer :: NESPEC`

Default value :: 6001

Description: Number of points used to calculate the dielectric function and other optical properties.

4.1.44 `real(kind=dp) :: CSHIFT`

Default value :: 0.01

Description: Smearing parameter used to avoid numerical singularities in the calculation of dielectric function including both real and imaginary parts. More details can be found in section 3.1.

4.1.45 `real(kind=dp) :: KTOL`

Default value :: 0.001

Description: Tolerance factor to avoid numerical singularities in the calculation of the Coulomb Potentials, used in BSE= T and BSE_BND= T calculations. More details can be in section 3.5.

4.1.46 `integer :: EXC_WF_I`

Default value :: 1

Description: First excitonic state to plot exciton wavefunction.

4.1.47 `integer ::  EXC_WF_F`

Default value :: 2

Description: Last excitonic state to plot exciton wavefunction. The excitonic wavefunctions are plot for the excitonic states in the interval `EXC_WF_I` to `EXC_WF_F`. (The highest excitonic state whose wavefunciton is plotted. The excitonic wavefunctions of the excitonic states in the interval `EXC_WF_I` to `EXC_WF_F` are plotted.

4.1.48 `character(len=5) ::  COULOMB_POT`

Default value :: V3D

Available values :: V3D, V3DL, V2DK, V2DT, V2DT2, V2DOH, V2DRK, V1DT, V0DT

Description: Selects the Coulomb potential which is used in `BSE= T` and `BSE_BND= T` calculations. More information about these potentials can be found in section 3.5.

4.1.49 `real(kind=dp) ::  EDIEL`

Default value :: 1.0

Description: Variable used to describe the Coulomb potentials. The more information can be found in section 3.5.

4.1.50 `real(kind=dp) ::  EDIEL_T`

Default value :: 1.0

Description: Variable used to describe the Coulomb potentials at finite temperature, more information can be found in section 3.5.

4.1.51 `real(kind=dp) ::  EDIEL_B`

Default value :: 1.0

Description: Variable used to describe the Coulomb potentials, more information can be found in section 3.5.

4.1.52 `real(kind=dp) :: EDIEL_Z`

Default value :: 1.0

Description: Variable used to describe the Coulomb potentials, more information can be found in section 3.5.

4.1.53 `real(kind=dp) :: W_COUL`

Default value :: 0.0

Description: Variable used to describe the Coulomb potentials, more information in section 3.5.

4.1.54 `real(kind=dp) :: LC`

Default value :: 1.0

Description: Variable used to describe the Coulomb potentials, more information in section 3.5.

4.1.55 `real(kind=dp) :: R_0`

Default value :: 1.0

Description: Variable used to describe the Coulomb potentials, more information in section 3.5.

4.1.56 `real(kind=dp) :: ST`

Default value :: 0.0

Description: Variable used in the finite temperature BSE. More information can be found in section 3.4.

4.1.57 `real(kind=dp) :: PHAVG`

Default value :: 0.0

Description: Variable used in the finite temperature BSE. More information can be found in section 3.4.

4.1.58 `real(kind=dp) :: TEMP`

Default value :: 0.0

Description: Temperature in K used in the finite temperature BSE. More information can be found in section3.4.

4.1.59 `character(len=6) :: SES`

Default value :: AM15G

Available values :: AM15G,AM15D,AM0G

Description: Selection of the type of solar emission spectrum. More information can be found in section 3.8.

4.1.60 `real(kind=dp) :: CTEMP`

Default value :: 298.15

Description: Solar cell Temperature in K used in the PCE calculation. More information can be found in section 3.8.

4.1.61 `real(kind=dp) :: THMAX`

Default value :: 5E-06

Description: Maximum solar cell thickness in m for PCE, with SLME method calculation. More information can be found in section 3.8.

4.1.62 `real(kind=dp) :: EG`

Default value :: 0.0

Description: Fundamental bandgap in eV used in the PCE calculation. More information can be found in section 3.8.

4.1.63 `real(kind=dp) :: EGD`

Default value :: 0.0

Description: Optical bandgap (direct bandgap of allowed optical transition) in eV used in the PCE calculation. More information can be found in section 3.8.

4.1.64 `real(kind=dp) :: EGS`

Default value :: 0.0

Description: Exciton ground state energy in eV used in the PCE calculation. Usually it is the lowest energy value obtained from `BSE_BND= T` or `BSET_BND= T` calculations. If the materil is of a direct bandgap, this value could also be the lowest energy value of `BSE= T` or `BSET= T` simulations. More information can be found in section 3.8.

4.1.65 `real(kind=dp) :: EBGS`

Default value :: 0.0

Description: The ground state energy of bright exciton in eV used in the PCE calculation. It is obtained from the lowest bright exciton energy calculation with the flags `BSE= T` or `BSET= T`.More information can be found in section 3.8.

4.2 PARAMS_FILE

This file contains the Tight-Binding parameters obtained from Wannier functions (Wannier90 code). It is principle data needed to run any simulations in this code.

- First Line: Type of DFT calculation used to generated the wannier90_hr.dat output file (from Wannier90 code). There are the following options: `NP` for non-polarized calculation, `SP` for spin polarized calculation and `SOC` for calculations considering spin-orbit coupling.

- Second Line: scissors operator used to correct bandgap, if necessary.

- Third Line: Fermi level energy, obtained in DFT calculation.

- Fourth Line: first lattice vector coordinates in real space

```
SOC
    0.00                              !scissors operator
   -1.2008                            !efermi
     3.1321841        0.0000000        0.0000000
    -1.5660921        2.7125510        0.0000000
     0.0000000        0.0000000       24.0000000
written on   4Sep2020 at 08:46:41
         22
        147
    1    1    1    1    1    2    1    1    1    1    1    2    1    1    1
    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
    1    1    1    1    1    1    1    2    1    1    1    1    1    1    1
    1    1    1    1    2    1    1    1    1    1    1    1    1    1    1
    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1
    2    1    1    1    1    1    2    1    1    1    1    1
   -8   -4    0    1    1     0.000065    -0.000000
   -8   -4    0    2    1    -0.000000    -0.000000
   -8   -4    0    3    1     0.000000     0.000000
   -8   -4    0    4    1    -0.000002     0.000000
   -8   -4    0    5    1    -0.000000    -0.000001
```

Figure S2: Example of `PARAMS_FILE`.

- Fifth Line: second lattice vector coordinates in real space

- Sixth Line: third lattice vector coordinates in real space

- Other Lines: wannier90_hr.dat file, outputted from Wannier90 code. For spin polarized calculation you add both spin up and down hr files, in this order.

The Wannier90 parameter's output file `wannier90_hr.dat` need to be generated using the flag `use_ws_distance=.false.` to assure correct results in our code.

4.3 ORB_W

This file serves as a tool to select the orbitals from the Hamiltonian basis set. "1" means the orbital being selected, while "0" denote that the orbital will not be used to obtain PDOS and **k**-resolved band structure with the contributions with the selected orbitals. The number of lines of this file is the same of the projections used to wannierize the DFT Hamiltonian.

The basis set order are informed in the `wannier90.nnkp` file, generated by the Wannier90 code.

If this file was not declared in input file, the code automatically considers all lines equals to 1.

Figure S3: Example of `ORB_W` file.

4.4 KPATH_FILE

Figure S4: Example of `KPATH_FILE`.

- First Line: Number of declared **k**-points to define the **k**-path, this value must be ≥ 2

- Second Line: Number of **k**-points per line-segment

- Other Lines: Declared **k**-points using direct coordinates of the reciprocal lattice vectors

The `KPATH_BSE` file are written exactly in the same format, however due the BSE computational cost, it's recommended to lower the number of intersections declared in the second line.

5 Output Files

In this section we'll explain the information written in all output files and provide an example of each one of them.

5.1 Log Files

5.1.1 log.dat

This file is generated each time you run the code, contains all parameters used in the calculation, the parameters not defined by the user, are showed their default values. This file also allows the user to see the progress of the selected calculations and how much times it cost.

Figure S5: Example of `log.dat`.

5.1.2 log_bse-diel.dat

This file is generated from `BSE= T` or `BSET= T` calculation, shows some specific parameters used in BSE calculation and the calculation progress.

5.1.3 log_bse_kpath.dat

This file is generated from `BSE_BND= T` or `BSET_BND= T` calculation, is very similar to the previous file however shows the progress of the exciton band structure calculations.

5.2 Electronic Properties Files

5.2.1 bands.dat

This file was generated by the flag `BANDS= T`, and shows the band structure. The Fermi level are set at 0. This file was divided in 4 columns, by the following:

- Column 1: **k**-point parametrized in the selected **k**-path in the interval of 0 to 1,

```
threads:          10

grid:          33              33               1

ktol-coulomb:    0.1000E-02

kmesh shift:        0.0000         0.0000         0.0000

conduction bands, nc:          1   valence bands, nv:          1


begin  day          19         11 hours        50 min        55 seg

direct gap:   2.19365717927109
eigenvalues and eigenvectors calculated
quantum numbers for exciton basis set finished
single particle optics finished
exciton Hamiltonian matrix finished
exciton Hamiltonian diagonalized
exciton ground state   1.77158898577046
xx tensor component
yy tensor component
zz tensor component
xy tensor component set to 0
xz tensor component set to 0
yz tensor component set to 0
sp polarization
sm polarization
optics finished


end   day          19         11 hours        50 min        56 seg
```

Figure S6: Example of `log_bse-diel.dat`.

```
threads:          10

grid:          33              33               1

ktol-coulomb:  1.000000047497451E-003

kmesh shift:  0.000000000000000E+000  0.000000000000000E+000
  0.000000000000000E+000

conduction bands, nc:          1   valence bands, nv:          1

number of kpoints in the path:              4


begin  day          19         11 hours        50 min        56 seg

quantum numbers for exciton basis set finished
progress:          1 /          4
progress:          2 /          4
progress:          3 /          4
progress:          4 /          4

end   day          19         11 hours        51 min         0 seg
```

Figure S7: Example of `log_bse_kpath.dat`.

- Column 2: Energy values in eV,

- Column 3: S_z average value, if your parameters are generated from non-polarized calculation NP in PARAMS_FILE, desconsider the values in these column,

- Column 4: Contribution from the selected orbital set, defined in ORB_W file.

#band	1		
0.0000000E+00	-6.724803	-0.1375256	1.000000
6.8034013E-03	-6.721933	0.4846156	1.000000
1.3606803E-02	-6.713345	0.9314451	1.000000
2.0410204E-02	-6.699100	0.9965844	1.000000
2.7213605E-02	-6.679298	0.9994529	1.000000
3.4017008E-02	-6.654092	0.9992782	1.000000
4.0820409E-02	-6.623687	0.9994917	1.000000
4.7623809E-02	-6.588350	0.9997458	1.000000
5.4427210E-02	-6.548416	0.9998930	1.000000
6.1230611E-02	-6.504288	0.9999489	1.000000
6.8034016E-02	-6.456446	0.9999583	1.000000
7.4837416E-02	-6.405448	0.9999514	1.000000
8.1640817E-02	-6.351944	0.9999417	1.000000
8.8444218E-02	-6.296687	0.9999324	1.000000
9.5247619E-02	-6.240556	0.9999228	1.000000

Figure S8: Example of bands.dat.

5.2.2 KLABELS.dat

This file was generated by the flag BANDS= T and shows the values of the defined **k**-points, written in KPATH_FILE in the **k**-point parametrization of the **k**-path, written in one column.

5.2.3 dos.dat

This file was generated by the flag DOS= T, and shows the density of states (DOS), spinDOS, sumDOS and PDOS. The Fermi level are set at 0. This file was divided in 6 columns for SP and SOC calculations, and 4 to NP calculation, by the following:

- Column 1: Energy values in eV,

- Column 2: DOS,

- Column 3: sumDOS,

- Column 4: PDOS of the contribution from the selected orbital set, defined in `ORB_W` file, if `NP` calculation, spin up DOS calculation for the other cases,

- Column 5: spin down DOS calculation,

- Column 6: PDOS of the contribution from the selected orbital set, defined in `ORB_W` file.

```
#energy tdos sumdos updos dndos awdos
    -10.0000        0.0000        0.0000        0.0000        0.0000        0.0000
     -9.9967        0.0000        0.0000        0.0000        0.0000        0.0000
     -9.9933        0.0000        0.0000        0.0000        0.0000        0.0000
     -9.9900        0.0000        0.0000        0.0000        0.0000        0.0000
     -9.9867        0.0000        0.0000        0.0000        0.0000        0.0000
     -9.9833        0.0000        0.0000        0.0000        0.0000        0.0000
     -9.9800        0.0000        0.0000        0.0000        0.0000        0.0000
     -9.9767        0.0000        0.0000        0.0000        0.0000        0.0000
     -9.9733        0.0000        0.0000        0.0000        0.0000        0.0000
```

Figure S9: Example of `dos.dat` with `SOC` or `SP` calculation.

5.3 Optical Properties Files

5.3.1 sp_optics.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations. This file contains the oscillator force of each optical transition considering the selected conduction and valence bands. It's divided in 7 columns, as the following:

- Column 1: Transition Energy in eV,

- Column 2: $F_{x,x}^{c,v,\mathbf{k}}$

- Column 3: $F_{y,y}^{c,v,\mathbf{k}}$

- Column 4: $F_{z,z}^{c,v,\mathbf{k}}$

- Column 5: $F_{x,y}^{c,v,\mathbf{k}}$

- Column 6: $F_{x,z}^{c,v,\mathbf{k}}$

- Column 7: $F_{y,z}^{c,v,\mathbf{k}}$

This file is used, as an input, to calculated the dielectric function and other optical properties.

```
#  energy  xx  yy  zz  xy  xz  yz
      2.1937        4.8129          4.8137          0.0000         -0.0006          0.0000          0.0000
      2.1937        4.8128          4.8138          0.0000         -0.0006          0.0000          0.0000
      2.2841        4.2238          4.1577          0.0000          0.2848          0.0000          0.0000
      2.2841        4.4354          3.9919          0.0000         -0.1923          0.0000          0.0000
      2.2841        3.9253          4.4554          0.0000          0.1137          0.0000          0.0000
      2.2841        4.4352          3.9918          0.0000         -0.1923          0.0000          0.0000
      2.2841        4.2235          4.1578          0.0000          0.2847          0.0000          0.0000
      2.2841        3.9253          4.4554          0.0000          0.1136          0.0000          0.0000
```

Figure S10: Example of `sp_optics.dat`.

5.3.2 sp_optics-pol.dat

This file was generated by the flag `DIEL= T, BSE= T or BSET= T` calculations, using the flag `CPOL= T`. This file contains the oscillator force of each optical transition considering the selected conduction and valence bands, shows the results considering $\sigma_\pm$ circular light polarization. It's divided in 6 columns, as the following:

- Column 1: Transition Energy in eV,

- Column 2: $F_{x,x}^{c,v,\mathbf{k}}$

- Column 3: $F_{y,y}^{c,v,\mathbf{k}}$

- Column 4: $F_{z,z}^{c,v,\mathbf{k}}$

- Column 5: $F_{\sigma_+,\sigma_+}^{c,v,\mathbf{k}}$

- Column 6: $F_{\sigma_-,\sigma_-}^{c,v,\mathbf{k}}$

This file is used as an input, to calculate the dielectric function and other optical properties.

```
#  energy  xx  yy  zz  sp  sm
      2.1937        4.8129          4.8137          0.0000          0.0000          9.6266
      2.1937        4.8128          4.8138          0.0000          9.6265          0.0000
      2.2841        4.2238          4.1577          0.0000          0.0098          8.3717
      2.2841        4.4354          3.9919          0.0000          0.0102          8.4170
      2.2841        3.9253          4.4554          0.0000          0.0099          8.3708
      2.2841        4.4352          3.9918          0.0000          8.4168          0.0102
      2.2841        4.2235          4.1578          0.0000          8.3714          0.0098
```

Figure S11: Example of `sp_optics-pol.dat`.

5.3.3 sp_diel_AA.dat

This file was generated by the flag `DIEL= T, BSE= T or BSET= T` calculations, combined with `SPEC= T` flag, having one file for each component of the dielectric function, real $\varepsilon_{1,\alpha,\beta}(\omega)$ and

imaginary $\varepsilon_{2,\alpha,\beta}(\omega)$ parts, where AA= `xx,yy,zz,xy,xz,yz`. It's divided in 3 columns, as the following:

- Column 1: Photon Energy in eV,

- Column 2: Real Part $\varepsilon_{1,\alpha,\beta}(\omega)$

- Column 3: Imaginary Part $\varepsilon_{2,\alpha,\beta}(\omega)$

```
#  energy   real   imag
  0.0000000E+00    1.000000        0.0000000E+00
  5.0000002E-04    1.000000        0.0000000E+00
  1.0000000E-03    1.000000        0.0000000E+00
  1.5000000E-03    1.000000        0.0000000E+00
  2.0000001E-03    1.000000        0.0000000E+00
  2.4999999E-03    1.000000        0.0000000E+00
  3.0000000E-03    1.000000        0.0000000E+00
```

Figure S12: Example of `sp_diel_AA.dat`.

5.3.4   sp_diel-pol_A.dat

This file was generated by the flag DIEL= T, BSE= T or BSET= T calculations, combined with SPEC= T and CPOL= T flags, having one file for each component of the dielectric function, where A= `x,y,z,sp,sm`, where x,y,z corresponds to the components xx,yy,zz of the dielectric function and sp,sm the components $\sigma_+\sigma_+, \sigma_-\sigma_-$ respectively. It's divided in 3 columns, as the following:

- Column 1: Photon Energy in eV,

- Column 2: Real Part $\varepsilon_{1,\alpha,\beta}(\omega)$

- Column 3: Imaginary Part $\varepsilon_{2,\alpha,\beta}(\omega)$

The format is exactly the same of `sp_diel_AA.dat` file.

5.3.5 tm_coef.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `TMCOEF= T` flag. This file shows the oscillator force of each optical transition, identifying the bands and the **k**-point of each optical transition. It is divided in 13 columns, as the following:

- Column 1: k_x in Cartesian coordinates

- Column 2: k_y in Cartesian coordinates

- Column 3: k_z in Cartesian coordinates

- Column 4: Number of occupied states for the **k**-point in previous columns

- Column 5: Number of the conduction band of this transition

- Column 6: Number of the valence band of this transition

- Column 7: Transition Energy in eV

- Column 8: $F_{x,x}^{c,v,\mathbf{k}}$

- Column 9: $F_{y,y}^{c,v,\mathbf{k}}$

- Column 10: $F_{z,z}^{c,v,\mathbf{k}}$

- Column 11: $F_{x,y}^{c,v,\mathbf{k}}$

- Column 12: $F_{x,z}^{c,v,\mathbf{k}}$

- Column 13: $F_{y,z}^{c,v,\mathbf{k}}$

5.3.6 tm_coef-pol.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `TMCOEF= T` and `CPOL= T` flags. This file shows the oscillator force of each optical transition (considers circular light polarization), identifying the bands and the **k**-point of each optical transition. It is divided in 12 columns, as the following:

Figure S13: Example of `tm_coef.dat`.

- Column 1: k_x in Cartesian coordinates

- Column 2: k_y in Cartesian coordinates

- Column 3: k_z in Cartesian coordinates

- Column 4: Number of occupied states for the **k**-point in previous columns

- Column 5: Number of the conduction band of this transition

- Column 6: Number of the valence band of this transition

- Column 7: Transition Energy in eV

- Column 8: $F_{x,x}^{c,v,\mathbf{k}}$

- Column 9: $F_{y,y}^{c,v,\mathbf{k}}$

- Column 10: $F_{z,z}^{c,v,\mathbf{k}}$

- Column 11: $F_{\sigma_+,\sigma_+}^{c,v,\mathbf{k}}$

- Column 12: $F_{\sigma_-,\sigma_-}^{c,v,\mathbf{k}}$

Figure S14: Example of `tm_coef-pol.dat`.

5.3.7 sp_absorption_coef.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag. This file contains the absorption coefficient, obtained through the dielectric functions. It's divided in 7 columns, by the following:

- Column 1: Photon Energy in eV

- Column 2: $A_{x,x}(\omega)$

- Column 3: $A_{y,y}(\omega)$

- Column 4: $A_{z,z}(\omega)$

- Column 5: $A_{x,y}(\omega)$

- Column 6: $A_{x,z}(\omega)$

- Column 7: $A_{y,z}(\omega)$

5.3.8 sp_absorption_coef-pol.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` and `CPOL= T` flags. This file contains the absorption coefficient (considering circular light polarization), obtained through the dielectric functions. It's divided in 6 columns, by the following:

- Column 1: Photon Energy in eV

- Column 2: $A_{x,x}(\omega)$

- Column 3: $A_{y,y}(\omega)$

- Column 4: $A_{z,z}(\omega)$

- Column 5: $A_{\sigma_+,\sigma_+}(\omega)$

- Column 6: $A_{\sigma_-,\sigma_-}(\omega)$

5.3.9 sp_extinction_coef.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag.This file contains the extinction coefficient obtained through the dielectric functions. It's divided in 7 columns, by the following:

- Column 1: Photon Energy in eV

- Column 2: $\kappa_{x,x}(\omega)$

- Column 3: $\kappa_{y,y}(\omega)$

- Column 4: $\kappa_{z,z}(\omega)$

- Column 5: $\kappa_{x,y}(\omega)$

- Column 6: $\kappa_{x,z}(\omega)$

- Column 7: $\kappa_{y,z}(\omega)$

5.3.10 sp_extinction_coef-pol.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag.This file contains the extinction coefficient (considering circular light polarization), obtained through the dielectric functions. It's divided in 6 columns, by the following:

- Column 1: Photon Energy in eV

- Column 2: $\kappa_{x,x}(\omega)$

- Column 3: $\kappa_{y,y}(\omega)$

- Column 4: $\kappa_{z,z}(\omega)$

- Column 5: $\kappa_{\sigma_+,\sigma_+}(\omega)$

- Column 6: $\kappa_{\sigma_-,\sigma_-}(\omega)$

5.3.11 sp_reflectibility.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag. This file contains the reflectibility obtained through the dielectric functions. It's divided in 7 columns, by the following:

- Column 1: Photon Energy in eV

- Column 2: $R_{x,x}(\omega)$

- Column 3: $R_{y,y}(\omega)$

- Column 4: $R_{z,z}(\omega)$

- Column 5: $R_{x,y}(\omega)$

- Column 6: $R_{x,z}(\omega)$

- Column 7: $R_{y,z}(\omega)$

5.3.12 sp_reflectibility-pol.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` and `CPOL= T` flag. This file contains the reflectibility (considering circular light polarization), obtained through the dielectric functions. It's divided in 6 columns, by the following:

- Column 1: Photon Energy in eV

- Column 2: $R_{x,x}(\omega)$

- Column 3: $R_{y,y}(\omega)$

- Column 4: $R_{z,z}(\omega)$

- Column 5: $R_{\sigma_+,\sigma_+}(\omega)$

- Column 6: $R_{\sigma_-,\sigma_-}(\omega)$

5.3.13   sp_refractive_index.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag.This file contains the refractive index, obtained through the dielectric functions. It is divided in 7 columns, by the following:

- Column 1: Photon Energy in eV

- Column 2: $n_{x,x}(\omega)$

- Column 3: $n_{y,y}(\omega)$

- Column 4: $n_{z,z}(\omega)$

- Column 5: $n_{x,y}(\omega)$

- Column 6: $n_{x,z}(\omega)$

- Column 7: $n_{y,z}(\omega)$

5.3.14   sp_refractive_index-pol.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` and `CPOL= T` flags. This file contains the refractive index (considering circular light polarization), obtained through the dielectric functions. It is divided in 6 columns by the following:

- Column 1: Photon Energy in eV

- Column 2: $n_{x,x}(\omega)$

- Column 3: $n_{y,y}(\omega)$

- Column 4: $n_{z,z}(\omega)$

- Column 5: $n_{\sigma_+,\sigma_+}(\omega)$

- Column 6: $n_{\sigma_-,\sigma_-}(\omega)$

5.3.15 sp_en_loss_func.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag. This file contains the energy loss function obtained through the dielectric functions. It is divided in 7 columns, by the following:

- Column 1: Photon Energy in eV

- Column 2: $L_{x,x}(\omega)$

- Column 3: $L_{y,y}(\omega)$

- Column 4: $L_{z,z}(\omega)$

- Column 5: $L_{x,y}(\omega)$

- Column 6: $L_{x,z}(\omega)$

- Column 7: $L_{y,z}(\omega)$

5.3.16 sp_en_loss_func-pol.dat

This file was generated by the flag `DIEL= T`, `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` and `CPOL= T` flags. This file contains the energy loss function (considering circular light polarization), obtained through the dielectric functions. It is divided in 6 columns by the following:

- Column 1: Photon Energy in eV

- Column 2: $L_{x,x}(\omega)$

- Column 3: $L_{y,y}(\omega)$

- Column 4: $L_{z,z}(\omega)$

- Column 5: $L_{\sigma_+,\sigma_+}(\omega)$

- Column 6: $L_{\sigma_-,\sigma_-}(\omega)$

5.3.17 bz_act_A.dat

This file was generated by the flag `OPT_BZ= T`. Shows $\sum_{c,v} F_{\alpha,\beta}^{c,v,\mathbf{k}}$ for each $\mathbf{k}$-point in the mesh, having one file for each component of the oscillator force, where `A= x,y,z,sp,sm`, where x,y,z corresponds to the components xx, yy, zz of the dielectric function and sp, sm the components $\sigma_+\sigma_+, \sigma_-\sigma_-$ respectively. Its divided in 4 columns, as the following:

- Column 1: k_x in Cartesian coordinates

- Column 2: k_x in Cartesian coordinates

- Column 3: k_x in Cartesian coordinates

- Column 4: $\sum_{c,v} F_{\alpha,\beta}^{c,v,\mathbf{k}}$

5.3.18 dichroism.dat

This file was generated by the flag `OPT_BZ= T`. Shows the dichroism for each $\mathbf{k}$-point in the mesh. It is divided in 4 columns, as the following:

- Column 1: k_x in Cartesian coordinates

- Column 2: k_x in Cartesian coordinates

- Column 3: k_x in Cartesian coordinates

- Column 4: $\sum_{c,v} \frac{F_{\sigma_+,\sigma_+}^{c,v,\mathbf{k}} - F_{\sigma_-,\sigma_-}^{c,v,\mathbf{k}}}{F_{\sigma_+,\sigma_+}^{c,v,\mathbf{k}} + F_{\sigma_-,\sigma_-}^{c,v,\mathbf{k}}}$

5.4 Berry Curvature Files

5.4.1 berry_curv_bz.dat

This file was generated by the flag `BERRY_BZ= T`, and shows the total Berry curvature in the selected $\mathbf{k}$-mesh (Brillouin Zone). It's divided in 6 columns, as the following:

- Column 1: k_x in Cartesian coordinates

- Column 2: k_x in Cartesian coordinates

- Column 3: k_x in Cartesian coordinates

- Column 4: $\Omega_{y,z}(\mathbf{k})$

- Column 5: $\Omega_{x,z}(\mathbf{k})$

- Column 6: $\Omega_{x,y}(\mathbf{k})$

5.4.2 berry_curv_kpath.dat

This file was generated by the flag BERRY= T, and shows the total Berry curvature in the selected **k**-path through KPATH_FILE. It's divided in 4 columns, as the following:

- Column 1: **k**-point parametrized in the selected **k**-path in the interval of 0 to 1

- Column 2: $\Omega_{y,z}(\mathbf{k})$

- Column 3: $\Omega_{x,z}(\mathbf{k})$

- Column 4: $\Omega_{x,y}(\mathbf{k})$

5.5 Excitonic Properties Files

5.5.1 bse_opt_diel.dat

This file was generated by the flag BSE= T or BSET= T calculations. This file contains the oscillator force of each excitonic energy considering the selected conduction and valence bands. It's divided in 7 columns, as the following:

- Column 1: Exciton Energy in eV,

- Column 2: $F_{x,x}^{n,BSE}$

- Column 3: $F_{y,y}^{n,BSE}$

- Column 4: $F_{z,z}^{n,BSE}$

- Column 5: $F_{x,y}^{n,BSE}$

- Column 6: $F_{x,z}^{n,BSE}$

- Column 7: $F_{y,z}^{n,BSE}$

This file is used, as an input, to calculated the dielectric function and other optical properties considering excitonic effects. It has the same format of `sp_optics.dat`.

5.5.2   bse_opt_diel-pol.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `CPOL= T` flag. This file contains the oscillator force of each excitonic energy considering the selected conduction and valence bands, shows the results considering $\sigma_{\pm}$ circular light polarization. It's divided in 6 columns, as the following:

- Column 1: Exciton Energy in eV,

- Column 2: $F_{x,x}^{n,BSE}$

- Column 3: $F_{y,y}^{n,BSE}$

- Column 4: $F_{z,z}^{n,BSE}$

- Column 5: $F_{\sigma_+,\sigma_+}^{n,BSE}$

- Column 6: $F_{\sigma_-,\sigma_-}^{n,BSE}$

This file is used as an input, to calculate the dielectric function and other optical properties considering excitonic effects. It has the same format of `sp_optics-pol.dat`

5.5.3   bse_diel_AA.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag, having one file for each component of the dielectric function, real $\varepsilon_{1,\alpha,\beta}(\omega)$ and imaginary $\varepsilon_{2,\alpha,\beta}(\omega)$ parts, considering excitonic effects, where `AA= xx,yy,zz,xy,xz,yz`. It's divided in 3 columns, as the following:

- Column 1: Photon Energy in eV,

- Column 2: Real Part $\varepsilon_{1,\alpha,\beta}^{BSE}(\omega)$

- Column 3: Imaginary Part $\varepsilon_{2,\alpha,\beta}^{BSE}(\omega)$

The format is exactly the same of `sp_diel_AA.dat` file.

5.5.4 bse_diel-pol_AA.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` and `CPOL= T` flags, having one file for each component of the dielectric function, where `A= x,y,z,sp,sm`, where x,y,z corresponds to the components xx,yy,zz of the dielectric function and sp,sm the components $\sigma_+\sigma_+, \sigma_-\sigma_-$ respectively, with excitonic effects. It's divided in 3 columns, as the following:

- Column 1: Photon Energy in eV,

- Column 2: Real Part $\varepsilon_{1,\alpha,\beta}^{BSE}(\omega)$

- Column 3: Imaginary Part $\varepsilon_{2,\alpha,\beta}^{BSE}(\omega)$

The format is exactly the same of `sp_diel_AA.dat` file.

5.5.5 bse_absorption_coef.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag. This file contains the absorption coefficient, with excitonic effects, obtained through the dielectric functions. It's has the same format of `sp_absorption_coef.dat`.

5.5.6 bse_absorption_coef-pol.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` and `CPOL= T` flags. This file contains the absorption coefficient (considering circular light polarization), with excitonic effects, obtained through the dielectric functions. It's has the same format of `sp_absorption_coef-pol.dat`.

5.5.7 bse_extinction_coef.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag. This file contains the extinction coefficient, with excitonic effects, obtained through the dielectric functions. It's has the same format of `sp_extinction_coef.dat`.

5.5.8 bse_extinction_coef-pol.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` and `CPOL= T` flags. This file contains the extinction coefficient (considering circular light polarization), with excitonic effects, obtained through the dielectric functions. It's has the same format of `sp_extinction_coef-pol.dat`.

5.5.9 bse_reflectibility.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag. This file contains the reflectibility, with excitonic effects, obtained through the dielectric functions. It's has the same format of `sp_reflectibility.dat`.

5.5.10 bse_reflectibility-pol.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` and `CPOL= T` flags. This file contains the reflectibility (considering circular light polarization), with excitonic effects, obtained through the dielectric functions. It's has the same format of `sp_reflectibility-pol.dat`.

5.5.11 bse_refractive_index.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag. This file contains the refractive index, with excitonic effects, obtained through the dielectric functions. It's has the same format of `sp_refractive_index.dat`.

5.5.12 bse_refractive_index-pol.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` and `CPOL= T` flags. This file contains the refractive index (considering circular light polarization), with excitonic effects, obtained through the dielectric functions. It's has the same format of `sp_refractive_index-pol.dat`.

5.5.13 bse_en_loss_func.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` flag. This file contains the energy loss function, with excitonic effects, obtained through the dielectric functions. It's has the same format of `sp_en_loss_func.dat`.

5.5.14 bse_en_loss_func-pol.dat

This file was generated by the flag `BSE= T` or `BSET= T` calculations, combined with `SPEC= T` and `CPOL= T` flags. This file contains the energy loss function (considering circular light polarization), with excitonic effects, obtained through the dielectric functions. It's has the same format of `sp_en_loss_func-pol.dat`.

5.5.15 exciton_lifetime.dat

This file was generated by the flags `BSE= T` combined with `SPEC= T`. This file contains the exciton lifetime $\tau^n_{(1D,2D,3D),\alpha,\beta}$, in seconds. It's divided in 5 columns, as the following:

- Column 1: Exciton Energy in eV

- Column 2: $\tau^n_{(1D,2D,3D)}$ obtained by the sum of *xx*, *yy* and *zz* components of oscillator force

- Column 3: $\tau^n_{(1D,2D,3D),x,x}$

- Column 4: $\tau^n_{(1D,2D,3D),y,y}$

- Column 5: $\tau^n_{(1D,2D,3D),z,z}$

5.5.16 exciton_lifetime-pol.dat

This file was generated by the flags BSE= T combined with SPEC= T and CPOL= T flags. This file contains the exciton lifetime $\tau^n_{(1D,2D,3D),\alpha,\beta}$, in seconds. It's divided in 7 columns, as the following:

- Column 1: Exciton Energy in eV

- Column 2: $\tau^n_{(1D,2D,3D)}$ obtained by the sum of *xx*, *yy* and *zz* components of oscillator force

- Column 3: $\tau^n_{(1D,2D,3D),x,x}$

- Column 4: $\tau^n_{(1D,2D,3D),y,y}$

- Column 5: $\tau^n_{(1D,2D,3D),z,z}$

- Column 6: $\tau^n_{(1D,2D,3D),\sigma_+,\sigma_+}$

- Column 7: $\tau^n_{(1D,2D,3D),\sigma_-,\sigma_-}$

5.5.17 exc_wf_N.dat

This file was generated by the flags BSE= T or BSET= T combined with BSE_WF= T, and shows the wavefunctions of the direct excitons, generate one file for each excitonic state in the interval of the flags EXC_WF_I to EXC_WF_F, N is the number of the excitonic state. It's divided in 8 columns as the following:

- Column 1: Number of occupied states in **k**-point

- Column 2: k_x in Cartesian coordinates

- Column 3: k_y in Cartesian coordinates

- Column 4: k_z in Cartesian coordinates

- Column 5: Number of conduction band (c)

- Column 6: Number of valence band (v)

- Column 7: Real part of exciton wavefunction $A_{c,v,\mathbf{k},0}^{n}$

- Column 8: Imaginary part of exciton wavefunction $A_{c,v,\mathbf{k},0}^{n}$

```
# excitonic state           1
# exciton energy:   1.77158898577046
# number occupied states         14 (not valid for metallic systems)
# Number of conduction states        1
# Number of valence states          1
# Number of kpoints       1089
# nocpk kx ky kz nc nv re_wf imag_wf
      14      0.0000      0.0000      0.0000      15      14    -0.1913E-04    -0.1331E-04
      14      0.0000      0.0702      0.0000      15      14     0.4485E-05     0.9567E-04
      14      0.0000      0.1404      0.0000      15      14     0.2133E-03    -0.1245E-03
      14      0.0000      0.2106      0.0000      15      14    -0.6215E-04    -0.5430E-03
      14      0.0000      0.2808      0.0000      15      14     0.6594E-04    -0.5996E-03
      14      0.0000      0.3510      0.0000      15      14     0.4979E-03    -0.9944E-03
      14      0.0000      0.4212      0.0000      15      14     0.4150E-03     0.6148E-03
      14      0.0000      0.4913      0.0000      15      14     0.1251E-03     0.5402E-03
      14      0.0000      0.5615      0.0000      15      14    -0.4185E-03    -0.1512E-03
      14      0.0000      0.6317      0.0000      15      14     0.2573E-02    -0.1332E-02
      14      0.0000      0.7019      0.0000      15      14    -0.2712E-02     0.8299E-03
      14      0.0000      0.7721      0.0000      15      14     0.6095E-03    -0.4474E-03
```

Figure S15: Example of `exc_wf_N.dat`.

5.5.18 exc_wf_N_M.dat

This file was generated by the flags `BSE_BND= T` or `BSET_BND= T` combined with `BSE_WF= T`, and shows the wavefunctions of the direct and indirect excitons, in the $\mathbf{k}$-path, defined by `KPATH_BSE`. Generate one file for each excitonic state in the interval of the flags `EXC_WF_I` to `EXC_WF_F`, for each calculated $\mathbf{k}$-point. N is the number of the excitonic state and M is the $\mathbf{k}$-point number. It's divided in 8 columns as the following:

- Column 1: Number of occupied states in $\mathbf{k}$-point

- Column 2: k_x in Cartesian coordinates

- Column 3: k_y in Cartesian coordinates

- Column 4: k_z in Cartesian coordinates

- Column 5: Number of conduction band (c)

- Column 6: Number of valence band (v)

- Column 7: Real part of exciton wavefunction $A_{c,v,\mathbf{k},\mathbf{Q}}^{n}$

- Column 8: Imaginary part of exciton wavefunction $A_{c,v,\mathbf{k},\mathbf{Q}}^{n}$

Figure S16: Example of `exc_wf_N_M.dat`.

5.5.19 bands_bse.dat

This file was generated by the flag BSE_BND= T or BSET_BND= T, and shows the exciton band structure. This file was divided in 2 columns, by the following:

- Column 1: **k**-point parametrized in the selected **k**-path in the interval of 0 to 1,

- Column 2: Exciton energy values in eV,

5.5.20 KLABELS-BSE.dat

This file was generated by the flag BSE_BND= T or BSET_BND= T and shows the values of the defined **k**-points, written in KPATH_BSE in the **k**-point parametrization of the **k**-path, written in one column.

6 Power Conversion Efficiency Files

6.1 PCE-Limit-sp.dat

This file is generated by the flag PCE= T and shows the calculation of Shockley-Queisser Limit PCE and SLME Limit, in both case the absorbance is considered a Heaviside function, with values different than zero after EGD (EBGS for excitonic effects) flag.

6.2 PCE-Limit-bse.dat

Equal the previous file in Figure S17, but considering excitonic effects.

Figure S17: Example of `PCE-Limit-sp.dat`.

6.3 SLME-sp.dat

This file is generated by the flag `PCE= T` and shows the results of PCE dependency with crystal thickness obtained using SLME method.

Figure S18: Example of `SLME-sp.dat`.

- Column 1: Crystal Thickness in μm,

- Column 2: Power Conversion Efficiency in %,

- Column 3: Maximum output current density ($J(V_{max})$) in W/Vm^2,

- Column 4: Reverse saturation current density (J_0) in W/Vm^2,

- Column 5:Short circuit current density (J_{sc}) in W/Vm^2,

- Column 6: Voltage that maximizes J (V_{max}) in V,

- Column 7:Open Circuit Voltage (V_{oc}) in V,

- Column 8: Fill Factor (FF) in %,

6.4   SLME-bse.dat

Equal the previous file in Figure S18, but considering excitonic effects.

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