Optical Parameters from Tuning electronic and conductivity features of Multilayer WTe_2 using point defects

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We investigate electronic, optical and thermoelectric features of monolayer and multilayer 1T' WTe_2 by *abinitio* calculations based on spin-polarized denstiy functional theory (DFT). We used Vasp package [1, 2] for optical calculations, where the imaginary part of the dielectric constant (ε_2) can be obtained by a summation over empty states using the following equation:

$$\varepsilon_2^{\alpha\beta}(\omega) = \frac{4\pi^2 e^2}{\Omega} \lim_{q\to 0} \frac{1}{q^2} \sum_{c,v,\mathbf{k}} 2\omega_{\mathbf{k}} \delta(\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}} - \omega) \times \langle u_{c\mathbf{k}+e_\alpha \mathbf{q}} | u_{v\mathbf{k}} \rangle \langle u_{c\mathbf{k}+e_\beta \mathbf{q}} | u_{v\mathbf{k}} \rangle^* \quad (1)$$

Here, c and v represent the conduction and valence band states, and $u_{c\mathbf{k}}$ represents the periodicity of the wave function at the **k**-point, respectively. The real part of the dielectric constant (ε_1) can be obtained by the Kramers-Kronig transformation [3] as follows:

$$\varepsilon_1^{\alpha\beta}(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\epsilon_2^{\alpha\beta}(\omega')\omega'}{\omega'^2 - \omega^2 + i\eta} d\omega' \quad (2)$$

The total frequency dependent complex dielectric constant is then the sum of these two terms as $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$.

With the frequency dependent complex dielectric constant, we can calculate the optical conductivity ($\sigma_1(\omega)$), absorbance ($A(\omega)$), extinction coefficient ($k(\omega)$), refractive index ($n(\omega)$) according to: [4]

$$\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega) = -i\frac{\omega}{4\pi}\left[\varepsilon_1(\omega) + i\varepsilon_2(\omega) - 1\right] \quad (3)$$

$$A(\omega) = \frac{\omega}{c}\varepsilon_2(\omega)\Delta z \quad (4)$$

$$k(\omega) = \frac{1}{\sqrt{2}}\left\{\left[\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)\right]^{\frac{1}{2}} - \varepsilon_1(\omega)\right\}^{\frac{1}{2}} \quad (5)$$

$$n(\omega) = \frac{1}{\sqrt{2}}\left\{\left[\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)\right]^{\frac{1}{2}} + \varepsilon_1(\omega)\right\}^{\frac{1}{2}} \quad (6)$$

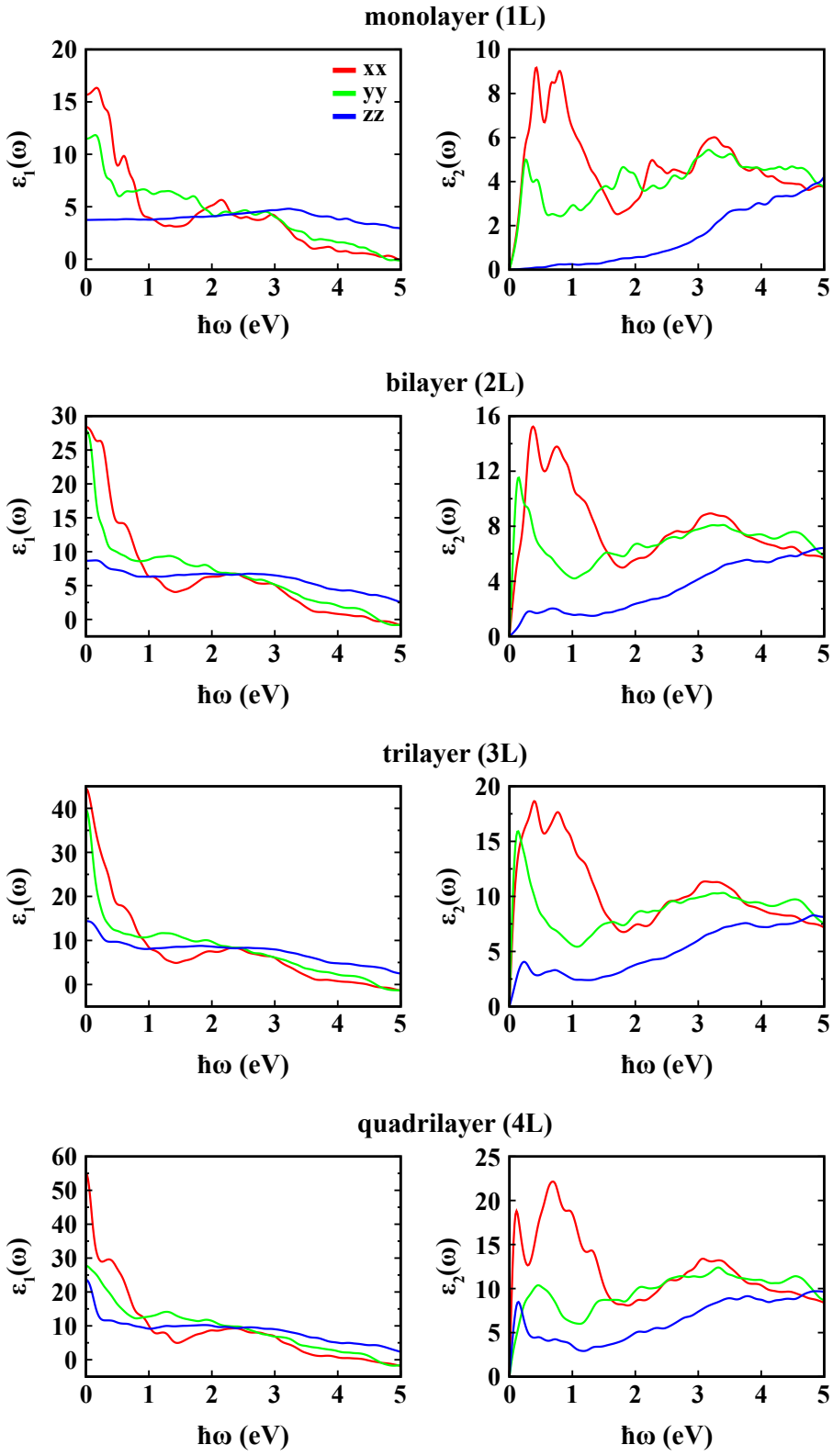

FIG. 1. Real ($\varepsilon_1(\omega)$) and imaginary ($\varepsilon_2(\omega)$) parts of frequency dependent dielectric constant calculated for 1L-to-4L 1T' WTe_2 as a function of photon energy ($\hbar\omega$) at 0 K along crystallographic axes (xx, yy, zz).

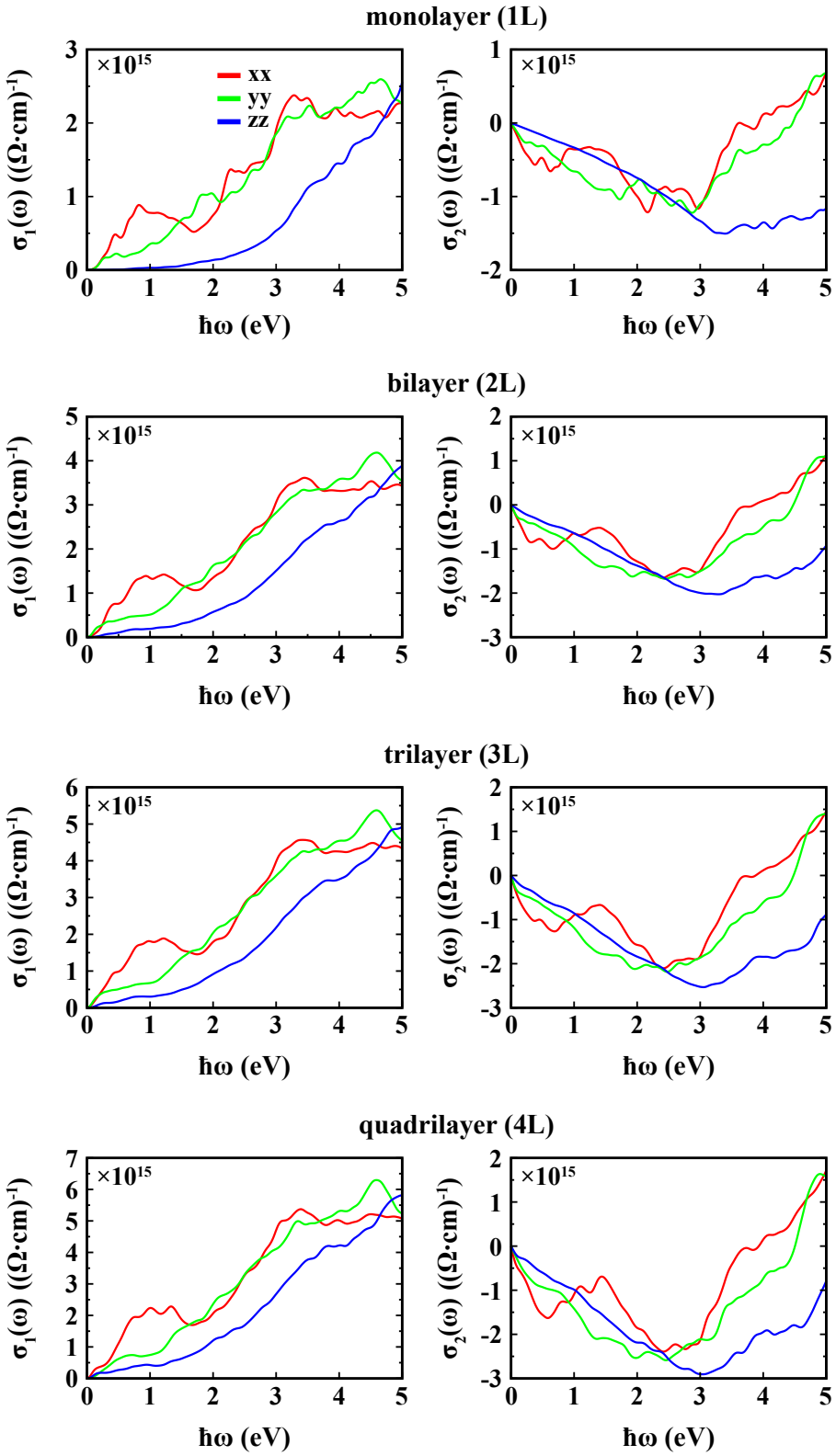

FIG. 2. Real ($\sigma_1(\omega)$) and imaginary ($\sigma_2(\omega)$) parts of frequency dependent optical conductivity calculated for 1L-to-4L 1T' WTe_2 as a function of photon energy ($\hbar\omega$) at 0 K along crystallographic axes (xx, yy, zz).

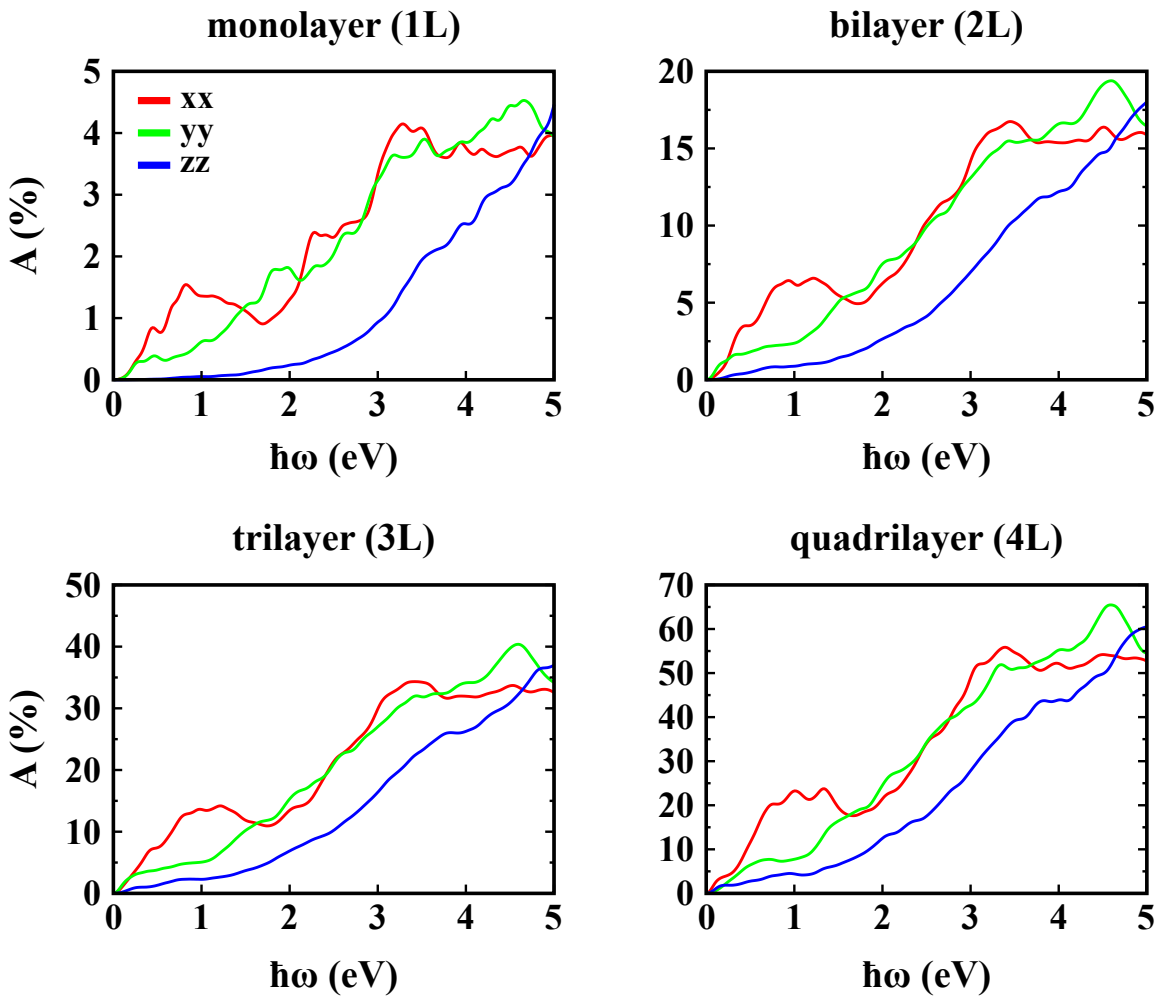

FIG. 3. Frequency dependent absorbance ($A(\omega)$) calculated for 1L-to-4L 1T' WTe_2 as a function of photon energy ($\hbar\omega$) at 0 K along crystallographic axes (xx, yy, zz).

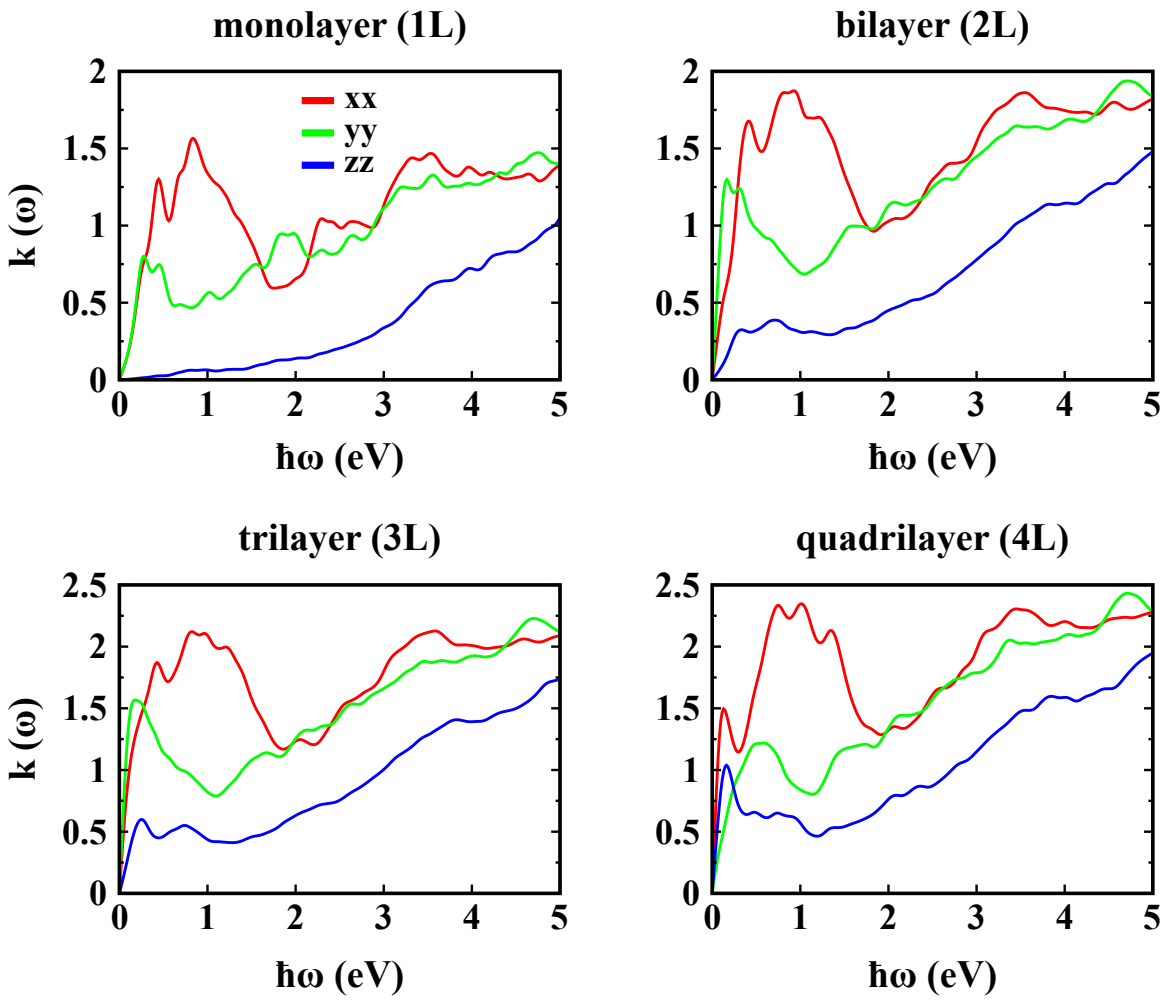

FIG. 4. Frequency dependent extinction coefficient ($k(\omega)$) calculated for 1L-to-4L 1T' WTe_2 as a function of photon energy ($\hbar\omega$) at 0 K along crystallographic axes (xx, yy, zz).

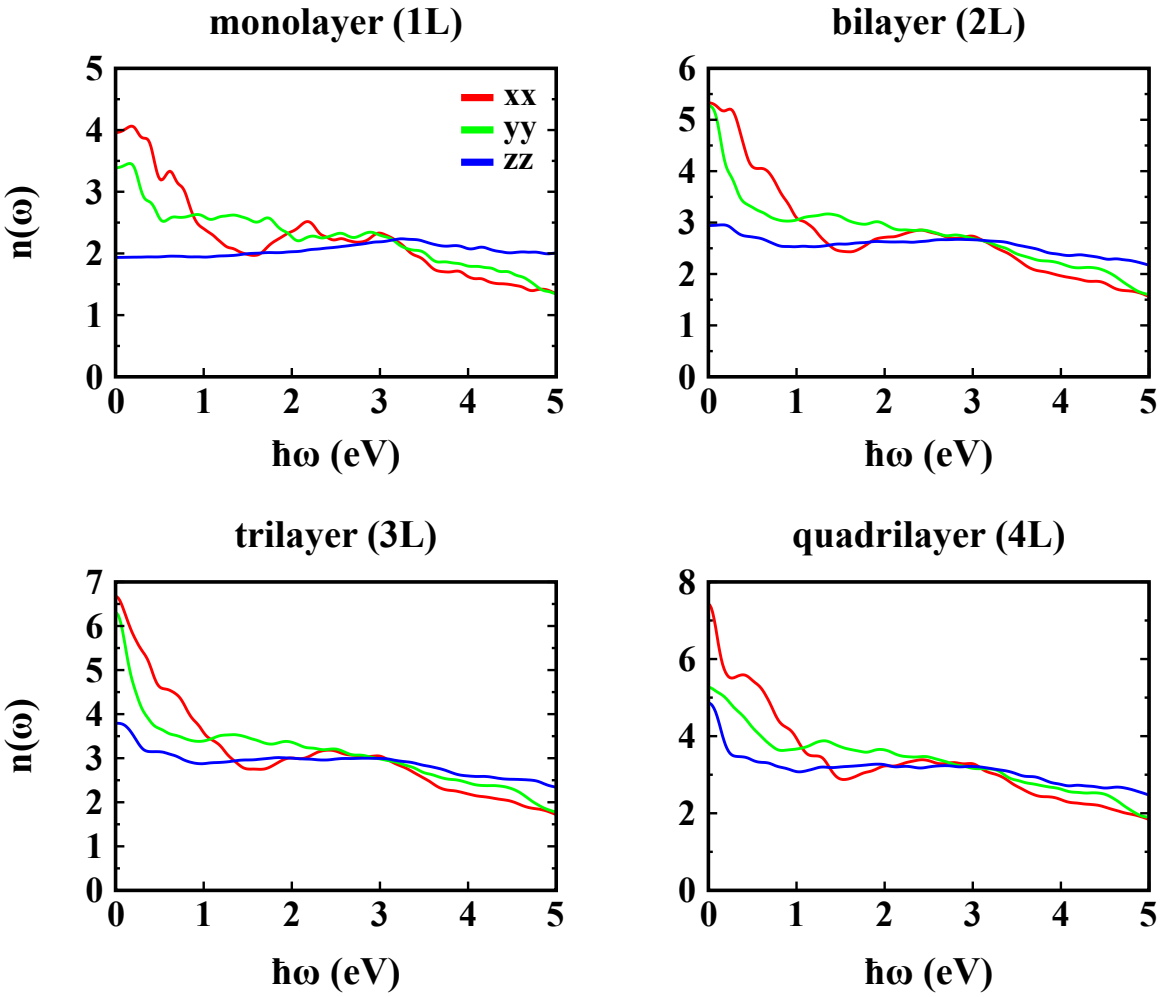

FIG. 5. Frequency dependent refractive index ($n(\omega)$) calculated for 1L-to-4L 1T' WTe_2 as a function of photon energy ($\hbar\omega$) at 0 K along crystallographic axes (xx, yy, zz).

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