Dielectric Function (ε):

The sum of the real and imaginary components of the incident photon energy is the complex dielectric function ε(ω), as seen in equation (1).

$$\varepsilon(\omega)=\varepsilon_1(\omega)+i\varepsilon_2(\omega) \tag{1}$$

The dielectric function are used to analyze the optical properties of any materials, it contains the real and imaginary parts which is shown in equation (1)

$$\varepsilon_2(\omega)=\left(\frac{4\pi e^2}{m^2\omega^2}\right)\sum_{i,j}\int_k \langle i \vee M \vee j \rangle^2 f_i(1-f_i)\delta(E_{j,k}-E_{i,k}-\omega)d^3k \tag{2}$$

where, M is the dipole matrix, i and j are the initial and final states respectively, f_i the Fermi distribution function for the i-th state, and E_i is the energy of electron in the i-th state with the crystal wave vector k. The real part $\varepsilon_1(\omega)$ of the dielectric function can be extracted from the imaginary part using the [22]

$$\varepsilon_1(\omega)=1+\frac{2}{\pi}P\int_0^\infty \frac{\omega'\varepsilon_2(\omega')d\omega}{\omega'^2-\omega^2} \tag{3}$$

Here, equation (2) use the formalism of Ehrenreich and Cohen and equation (3) can be derived from equation (2) with Kramerse-Kronig relation.

The knowledge of the both real ε1(ω) and the imaginary part ε2(ω) of the dielectric tensor with density functional perturbation theory (DFPT) allows the calculation of important optical functions such as the refractive index n(ω), extinction coefficient k(ω), absorption coefficient α(ω), conductivity σ(ω), reflectivity R(ω), and energy loss function L(ω), using the following expressions:

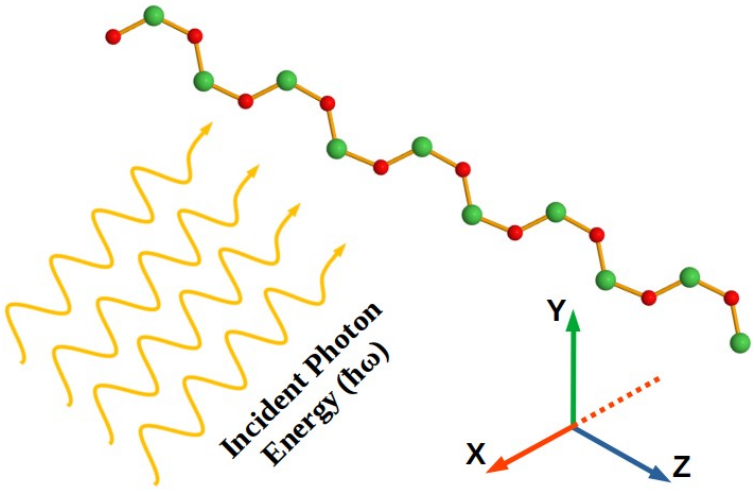

Figure 1: Model of Incident Photon Energy in single layer XO sheet.

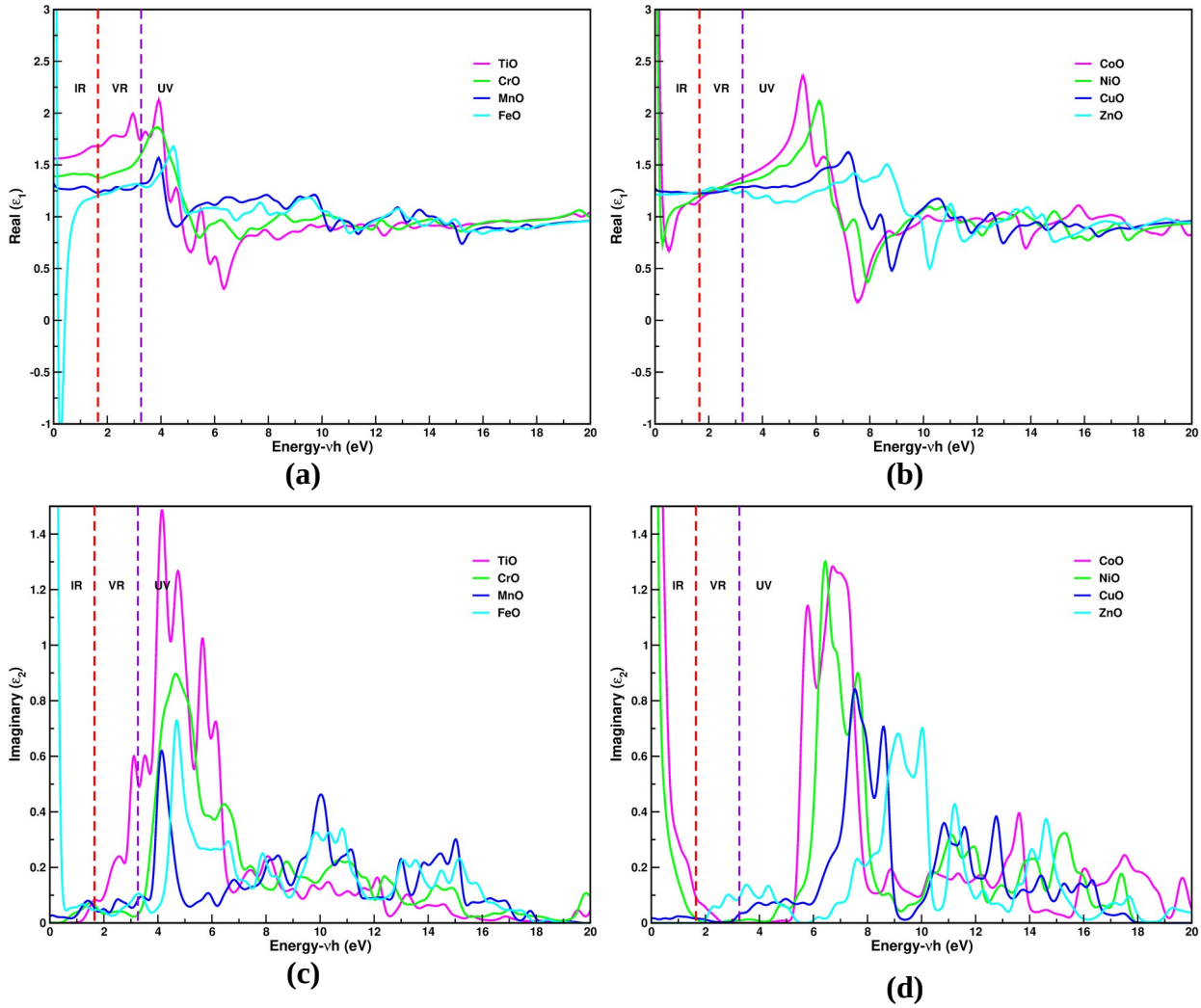

Figure 2. Dielectric functions of various single chain of d-block oxides Real (ε_1) part vs Energy plot of (a) TiO, CrO, MnO & FeO (b) CoO, NiO, CuO & ZnO and Imaginary (ε_2) part vs Energy plot of (c) TiO, CrO, MnO & FeO (d) CoO, NiO, CuO & ZnO

Refractive Index (n):

$$n(\omega)=\sqrt{\frac{\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}+\varepsilon_1(\omega)}{2}}$$

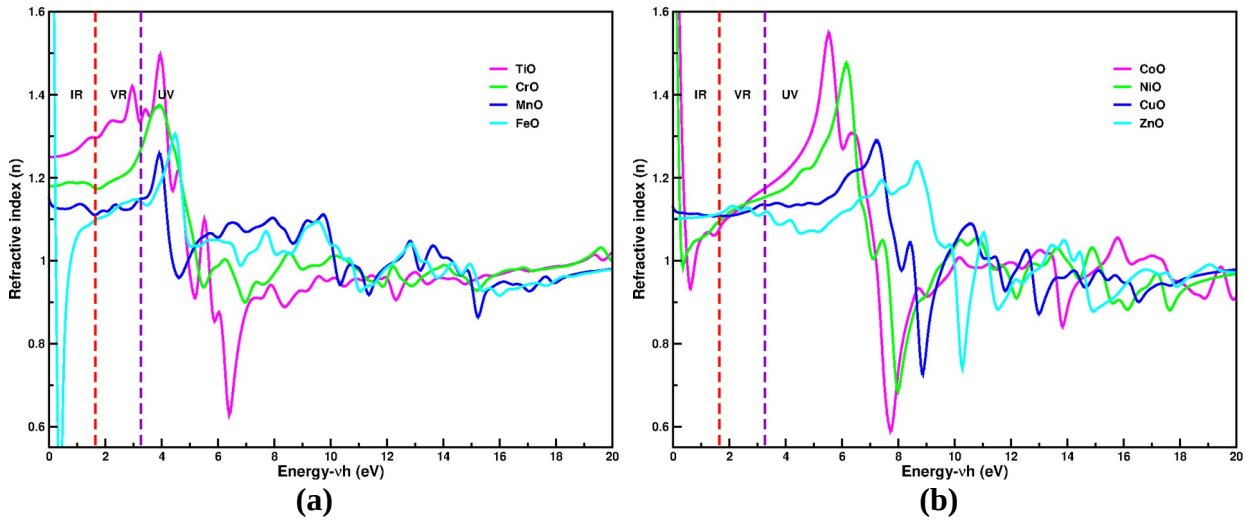

Figure 3. Refractive index (n) of various d-block oxides of (a) TiO, CrO, MnO & FeO (b) CoO, NiO, CuO & ZnO single chain

Extinction Coefficient k(ω):

$$k(\omega)=\sqrt{\frac{\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}-\varepsilon_1(\omega)}{2}}$$

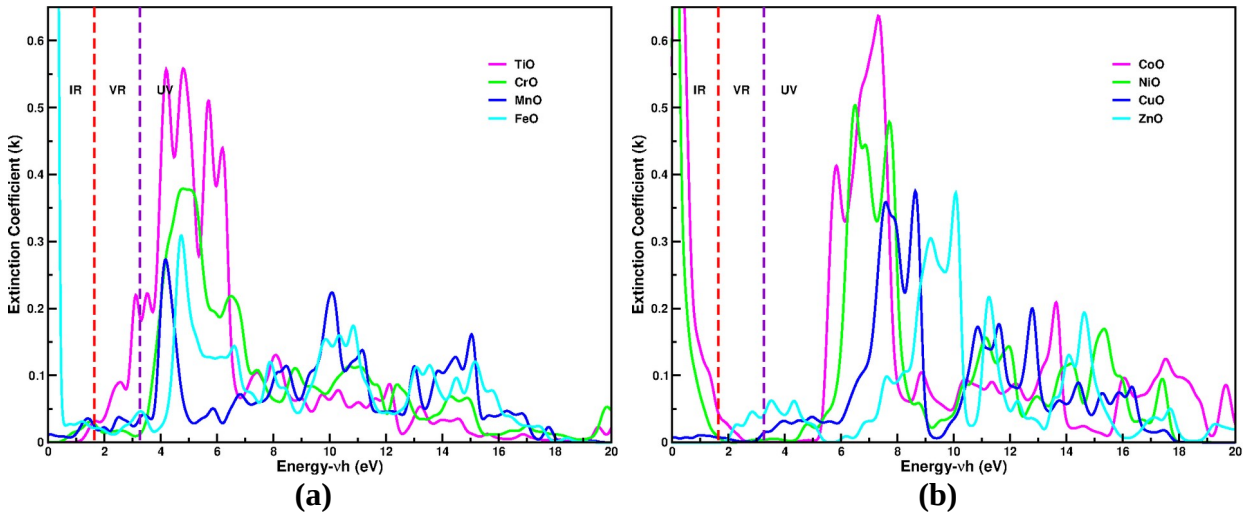

Figure 4. Extinction Coefficient (k) of various d-block oxides of (a) TiO, CrO, MnO & FeO (b) CoO, NiO, CuO & ZnO single chain

Absorption Coefficeint (α) :

$$\alpha(\omega)=\omega\sqrt{2\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}-2\varepsilon_1(\omega)}$$

$$\alpha(\omega)=\frac{4\pi k(\omega)}{\lambda}$$

$$\alpha(\omega)=\frac{2\omega k(\omega)}{c}$$

k(w) = extinction coefficient

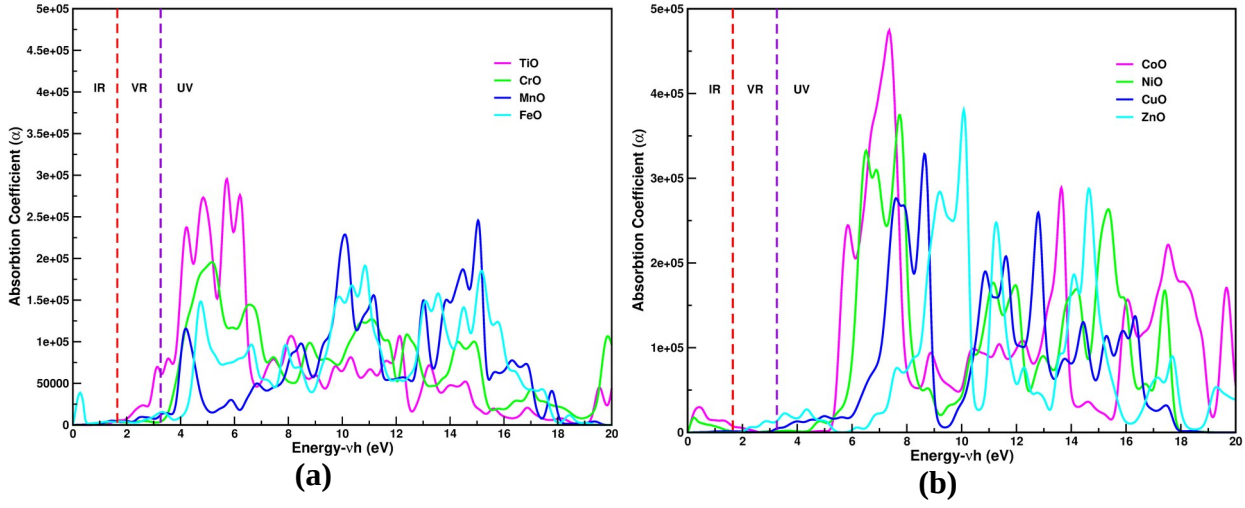

Figure 5. Absorption Coefficeint (α) of various d-block oxides of (a) TiO, CrO, MnO & FeO (b) CoO, NiO, CuO & ZnO single chain

Conductivity (σ) :

$$\sigma(\omega)=\frac{\omega\,\varepsilon_2(\omega)}{4\pi}$$

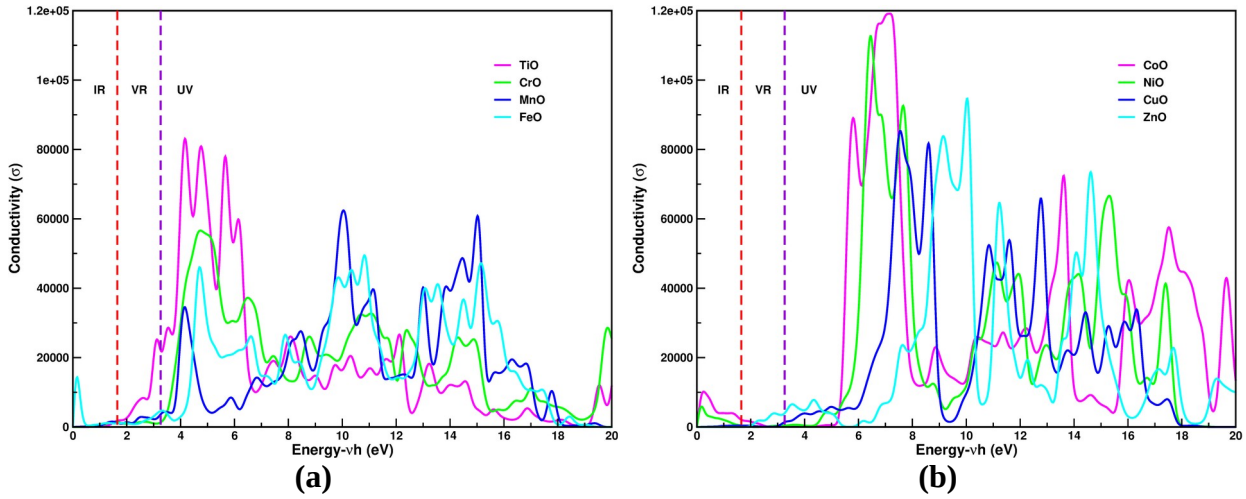

Figure 6. Conductivity (σ) of various d-block oxides of (a) TiO, CrO, MnO & FeO (b) CoO, NiO, CuO & ZnO single chain

Reflectance (R) :

$$R(\omega)=\left(\frac{\sqrt{\varepsilon(\omega)}-1}{\sqrt{\varepsilon(\omega)}+1}\right)^2$$

$$R(\omega)=\left(\frac{\sqrt{\varepsilon_1(\omega)+j\varepsilon_2(\omega)}-1}{\sqrt{\varepsilon_1(\omega)+j\varepsilon_2(\omega)}+1}\right)^2$$

$$R(\omega)=\frac{(1-n)^2+k^2}{(1+n)^2+k^2}$$

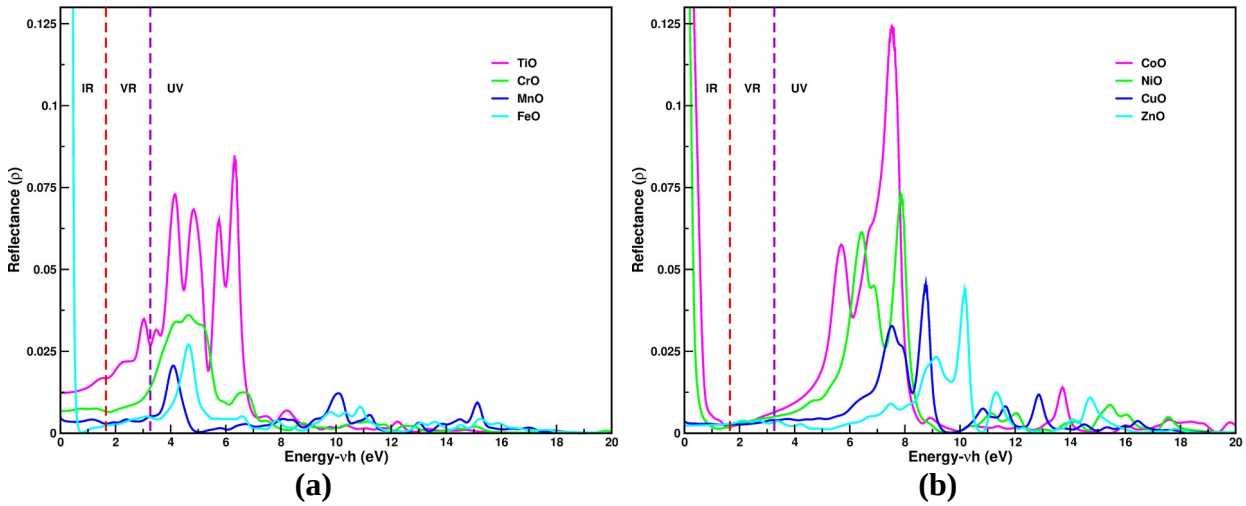

Figure 7. Reflectance (R) of various d-block oxides of (a) TiO, CrO, MnO & FeO (b) CoO, NiO, CuO & ZnO single chain

Energy Loss Function (L):

$$L(\omega)=\frac{\varepsilon_2(\omega)}{\varepsilon_1(\omega)+\varepsilon_2(\omega)}$$

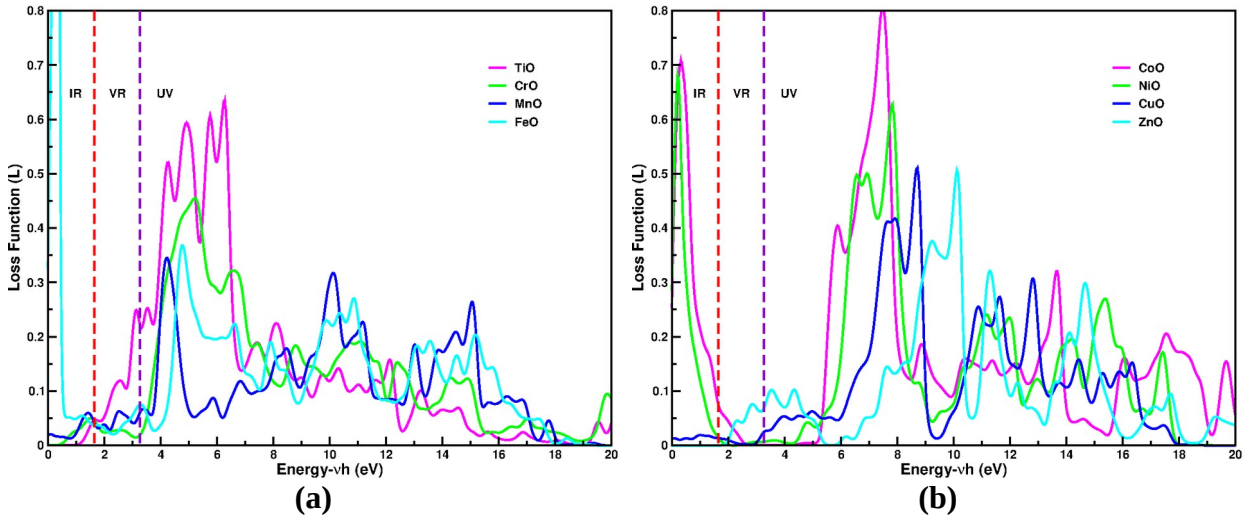

Figure 8. Energy loss function (L) of various d-block oxides of (a) TiO, CrO, MnO & FeO (b) CoO, NiO, CuO & ZnO single chain

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