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Electronic and optical properties of vanadium oxides from first principles

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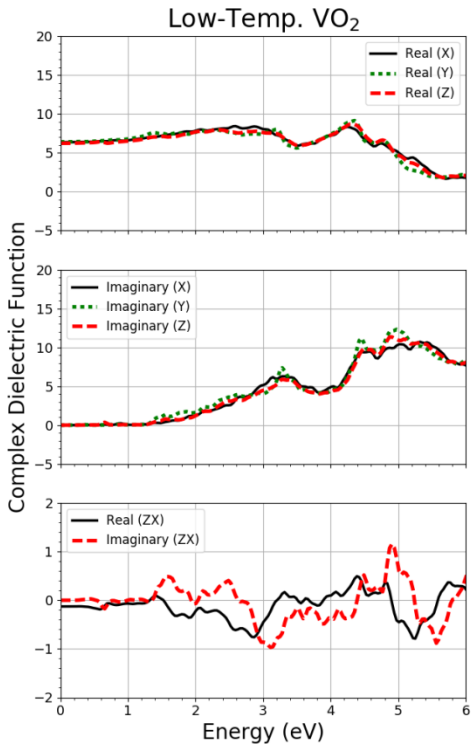
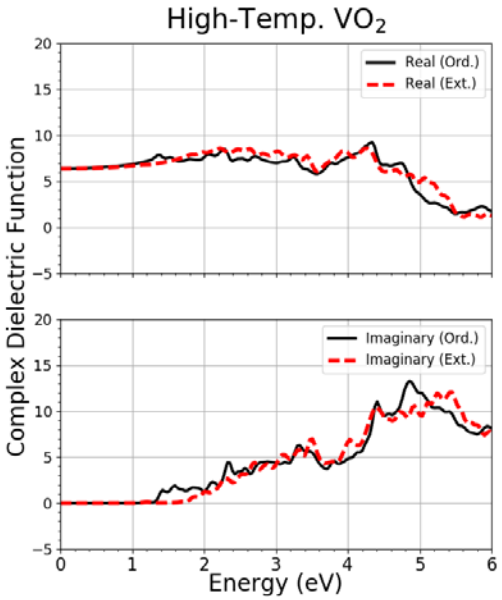
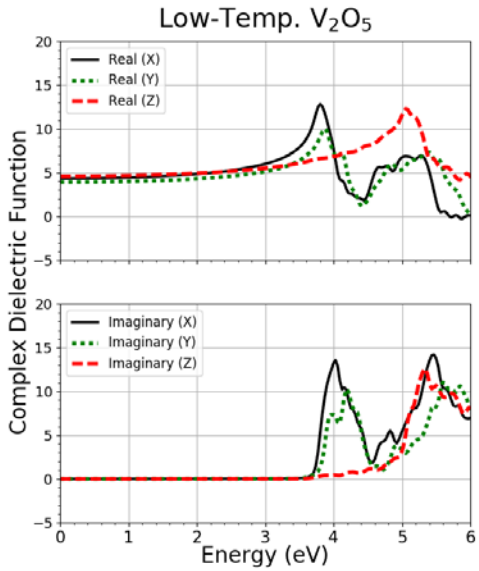
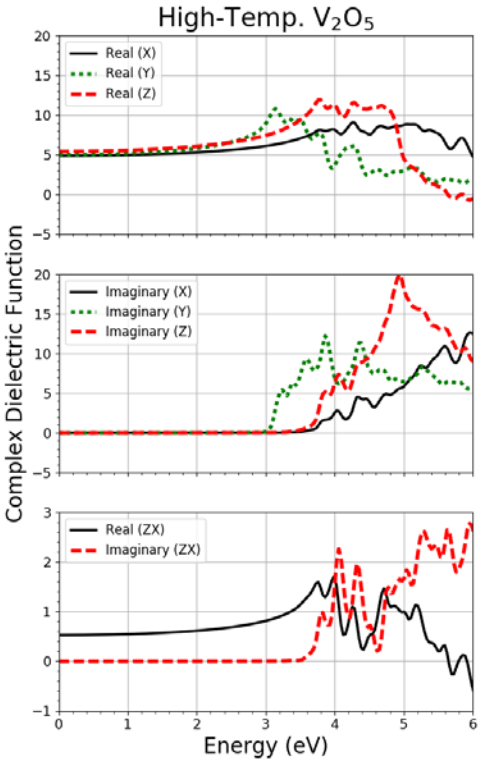
Table S1: The average values of charge transfer, in units of elementary electronic charge (-*e*), from vanadium to oxygen, along with the V-O ratio for each compound in the high- and low-temperature (LT and HT) phases.

Compound	Phase	V-O Ratio	Charge Transfer (-*e*)
VO_2	HT	1/2	0.9601
VO_2	LT	1/2	0.9597
V_2O_5	HT	2/5	1.1213
V_2O_5	LT	2/5	1.1250
V_2O_3	HT	2/3	0.8095
V_2O_3	LT	2/3	0.8537
V_3O_5	HT	3/5	0.8540
V_3O_5	LT	3/5	0.8548
V_4O_7	HT	4/7	0.8850
V_4O_7	LT	4/7	0.8878
V_6O_{13}	HT	6/13	1.0313
V_6O_{13}	LT	6/13	1.0273


Low-Temp. VO_2
Real (X)
Real (Y)
Real (Z)
Imaginary (X)
Imaginary (Y)
Imaginary (Z)
Real (ZX)
Imaginary (ZX)
Complex Dielectric Function
Energy (eV)


High-Temp. VO_2
Real (Ord.)
Real (Ext.)
Imaginary (Ord.)
Imaginary (Ext.)
Complex Dielectric Function
Energy (eV)


Low-Temp. V_2O_5
Real (X)
Real (Y)
Real (Z)
Imaginary (X)
Imaginary (Y)
Imaginary (Z)
Complex Dielectric Function
Energy (eV)


High-Temp. V_2O_5
Real (X)
Real (Y)
Real (Z)
Imaginary (X)
Imaginary (Y)
Imaginary (Z)
Real (ZX)
Imaginary (ZX)
Complex Dielectric Function
Energy (eV)

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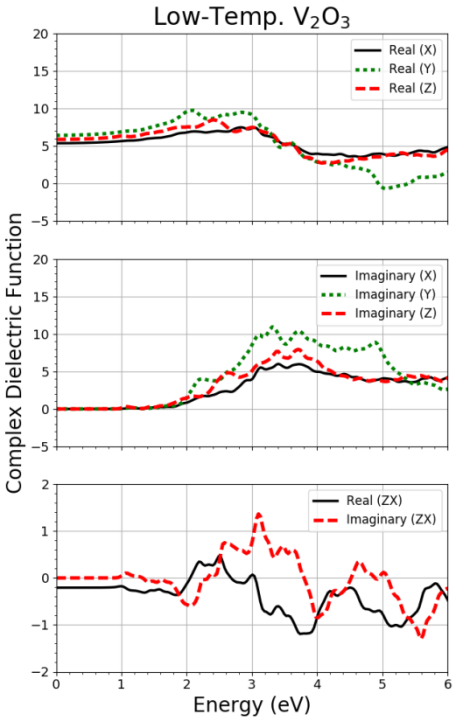

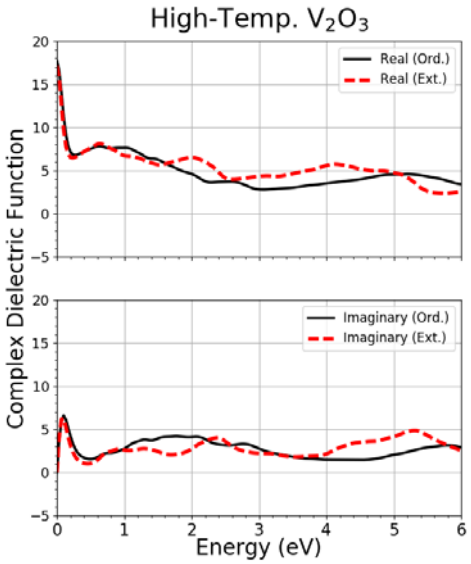

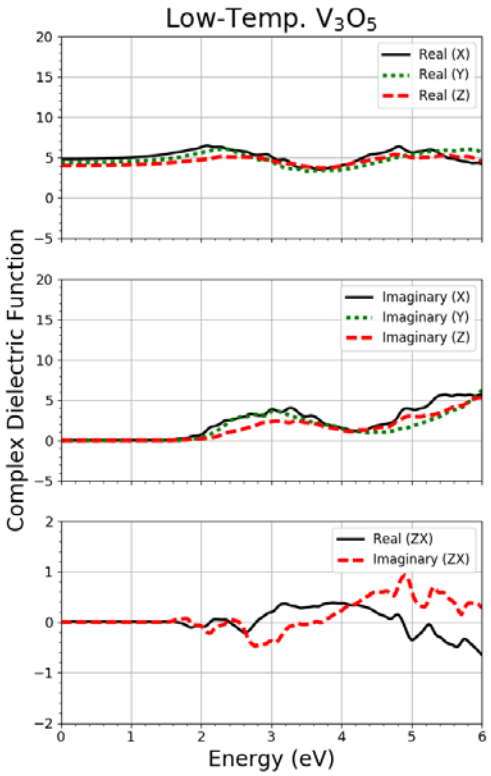

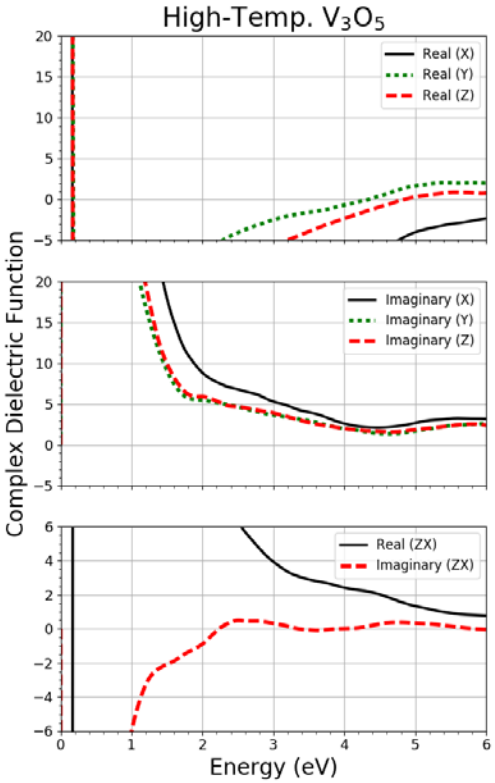

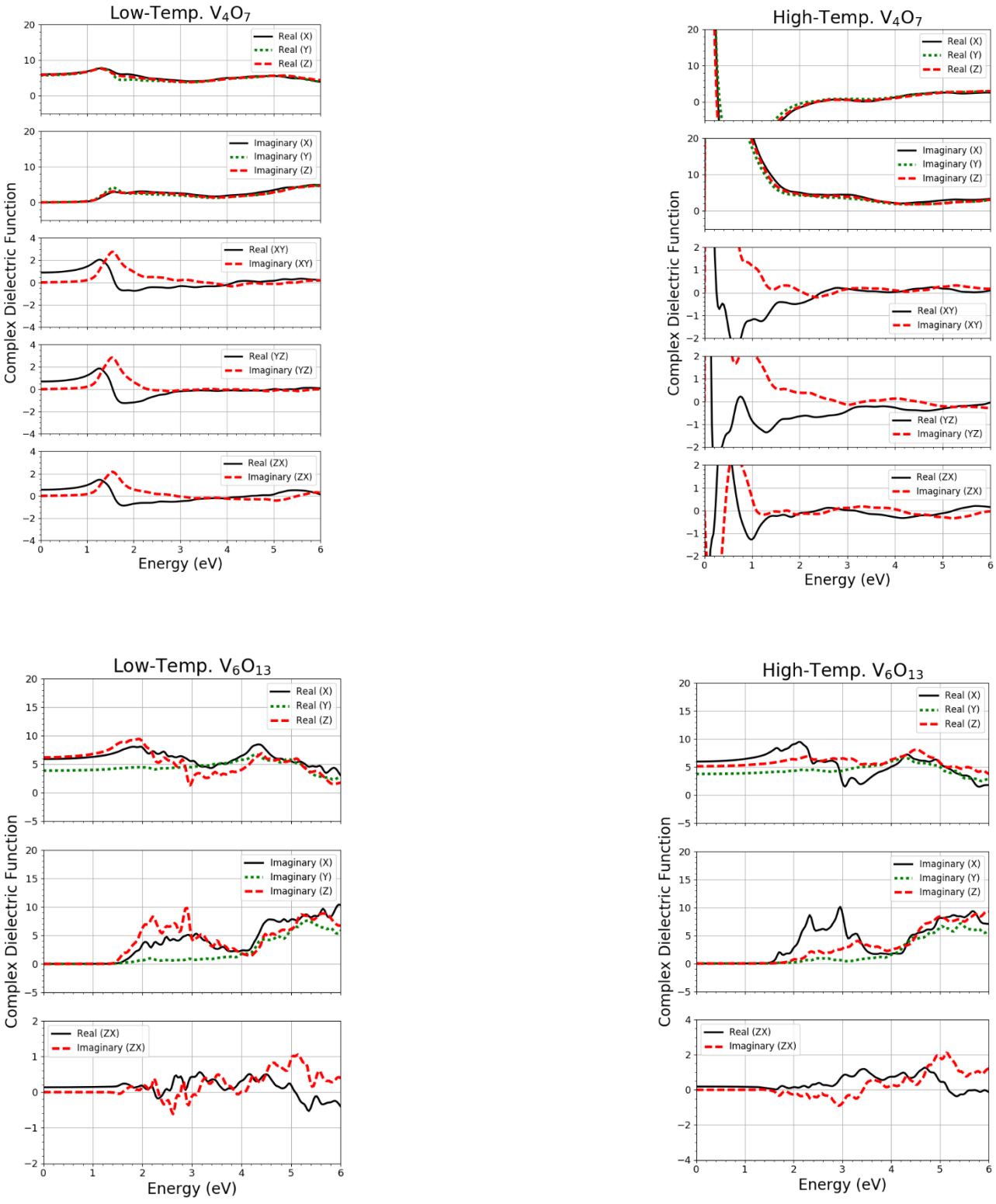

Figure S1: The real and imaginary parts of the complex dielectric function, as calculated through implementation of the hybrid HSE06 functional. Due to the anisotropic nature of the materials, we have plotted the dielectric values in each direction according to the level of anisotropy within the compound. For monoclinic and triclinic compounds, the off-diagonal components are also shown.

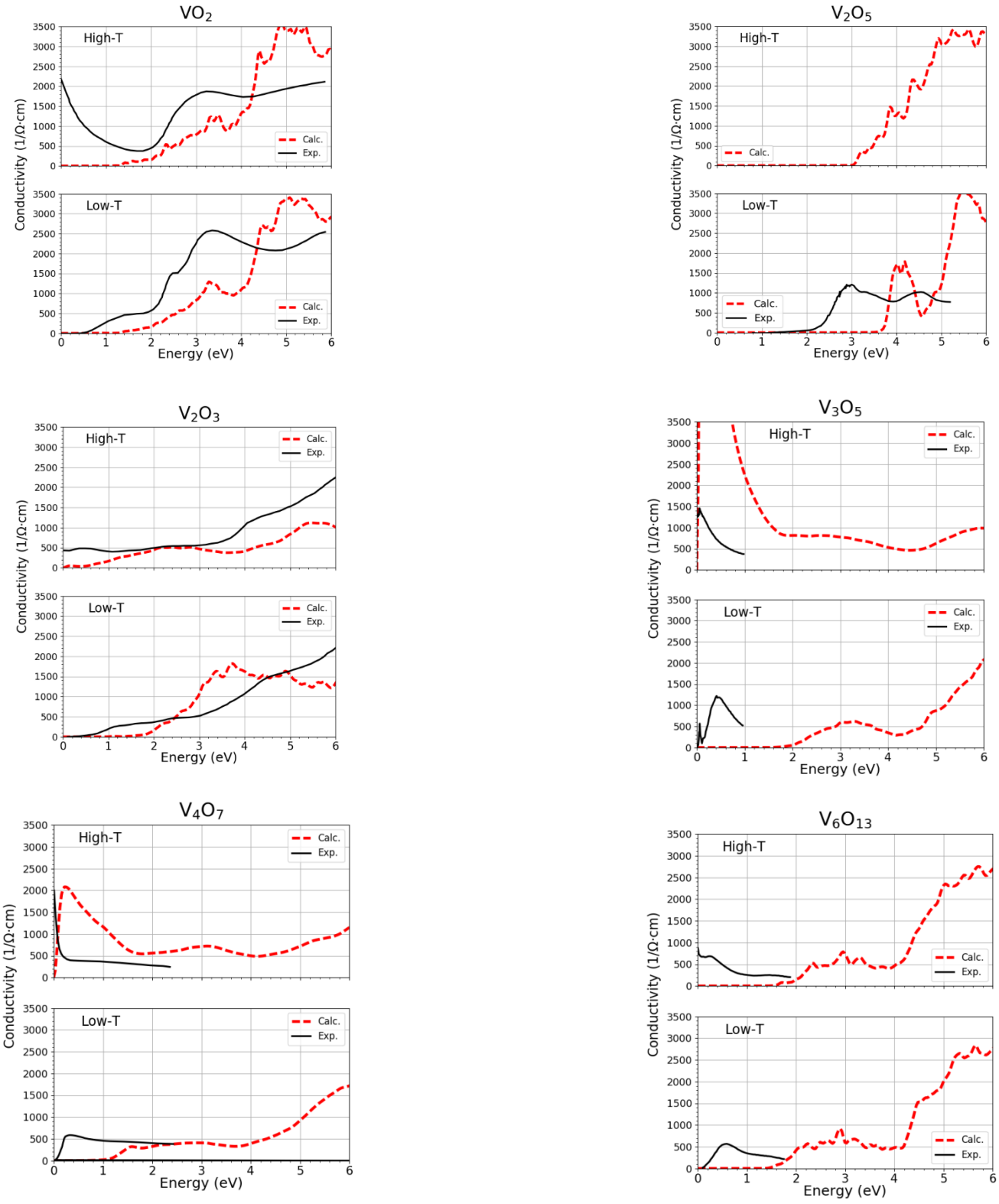

Figure S2: Optical conductivity of each compound, obtained through implementation of the hybrid HSE06 functional. Both the calculated and experimental results are plotted as a function of photon energy, ranging from 0 to 6 eV. Due to the anisotropic nature of the materials, we have calculated the average of the conductivity in the three dimensions and used these resulting values in order to compare with experimental data.

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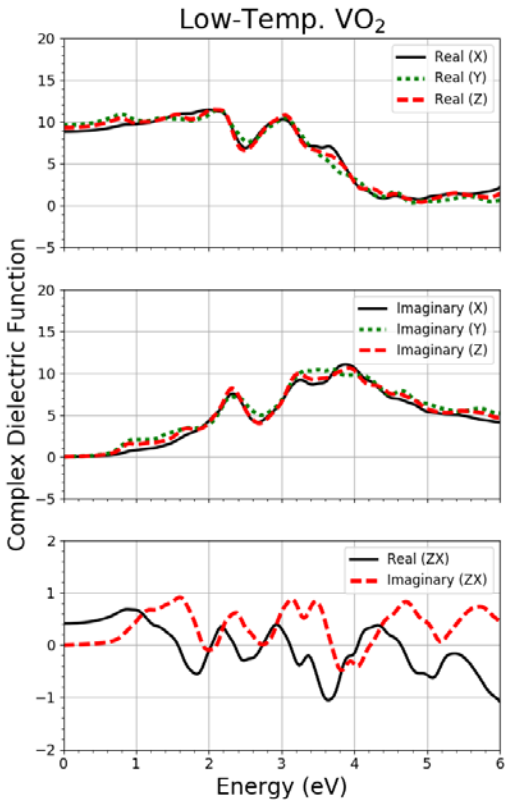

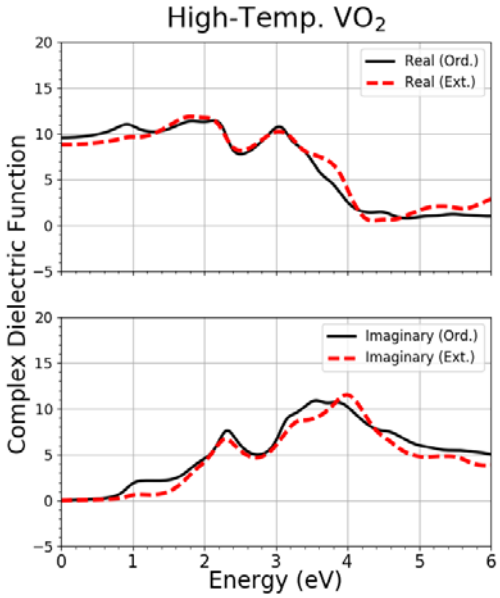

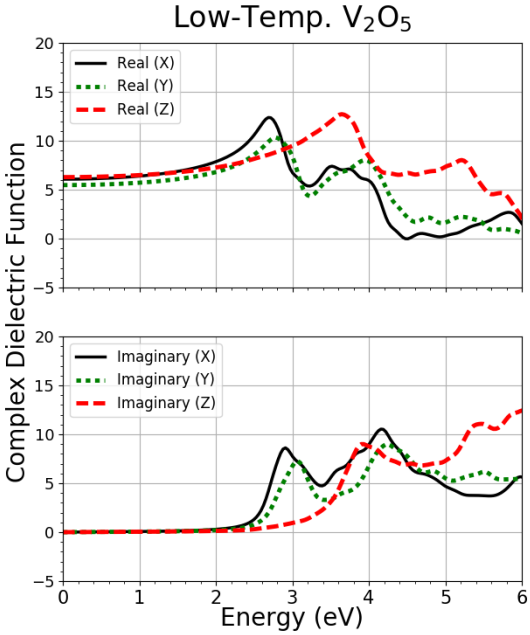

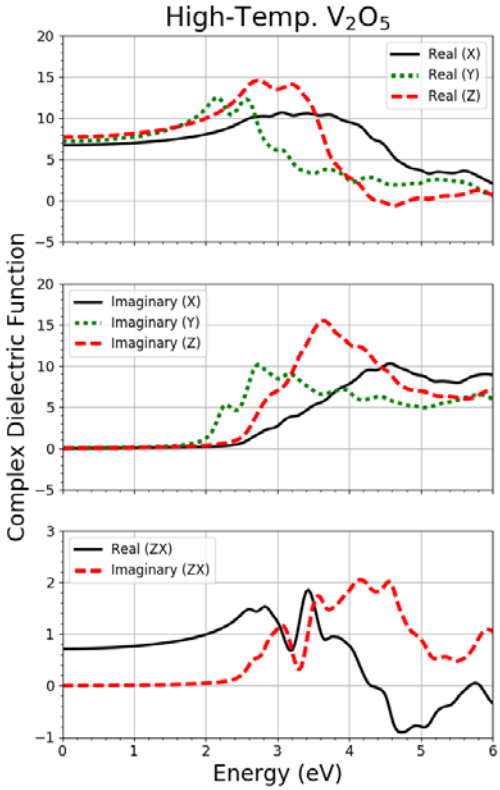

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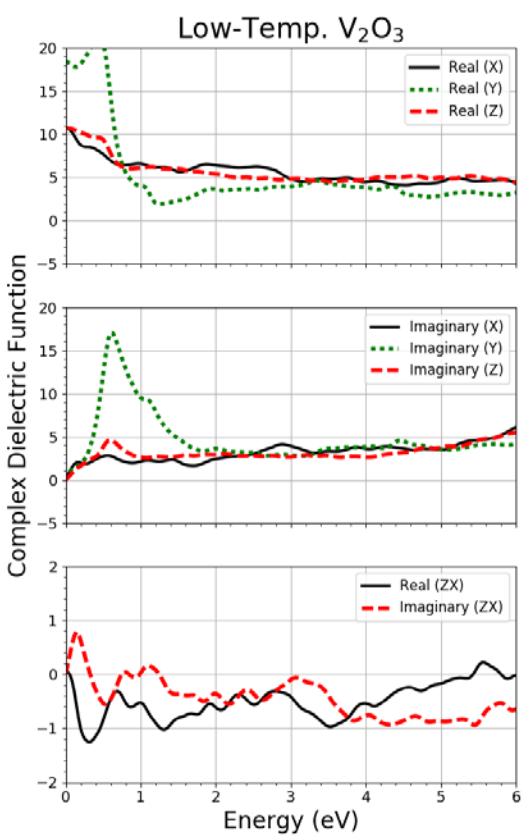

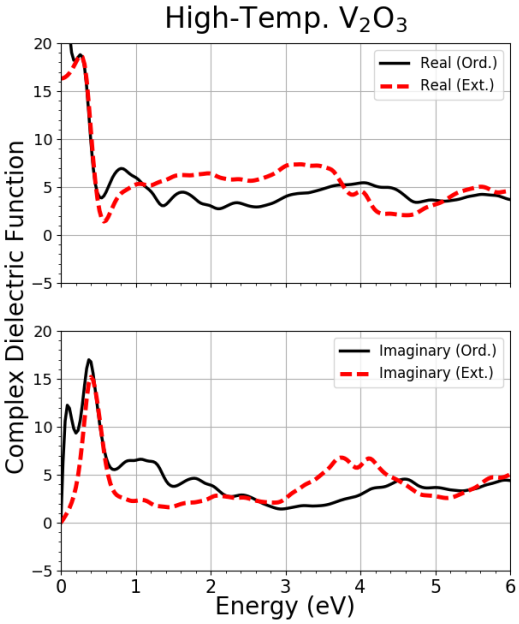

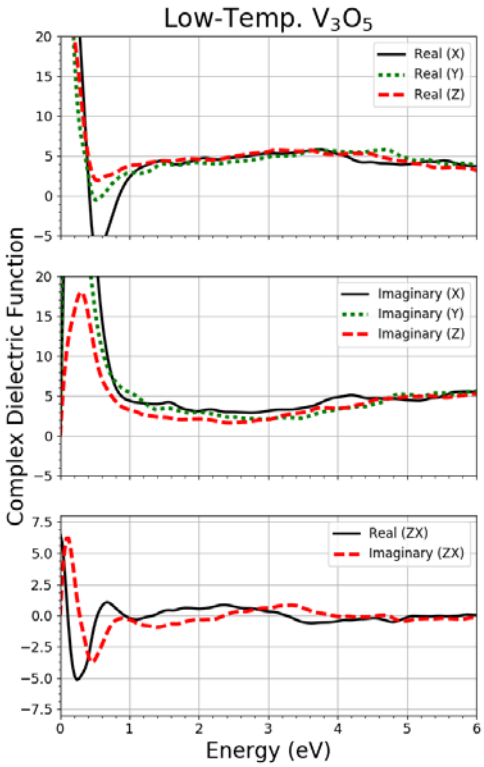

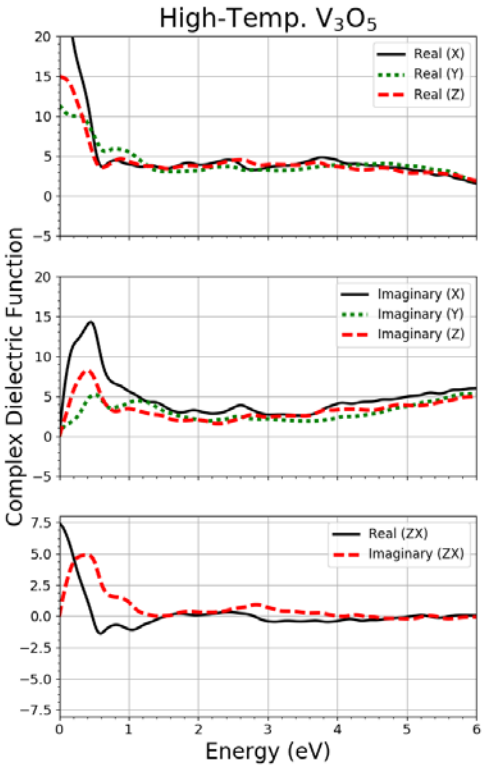

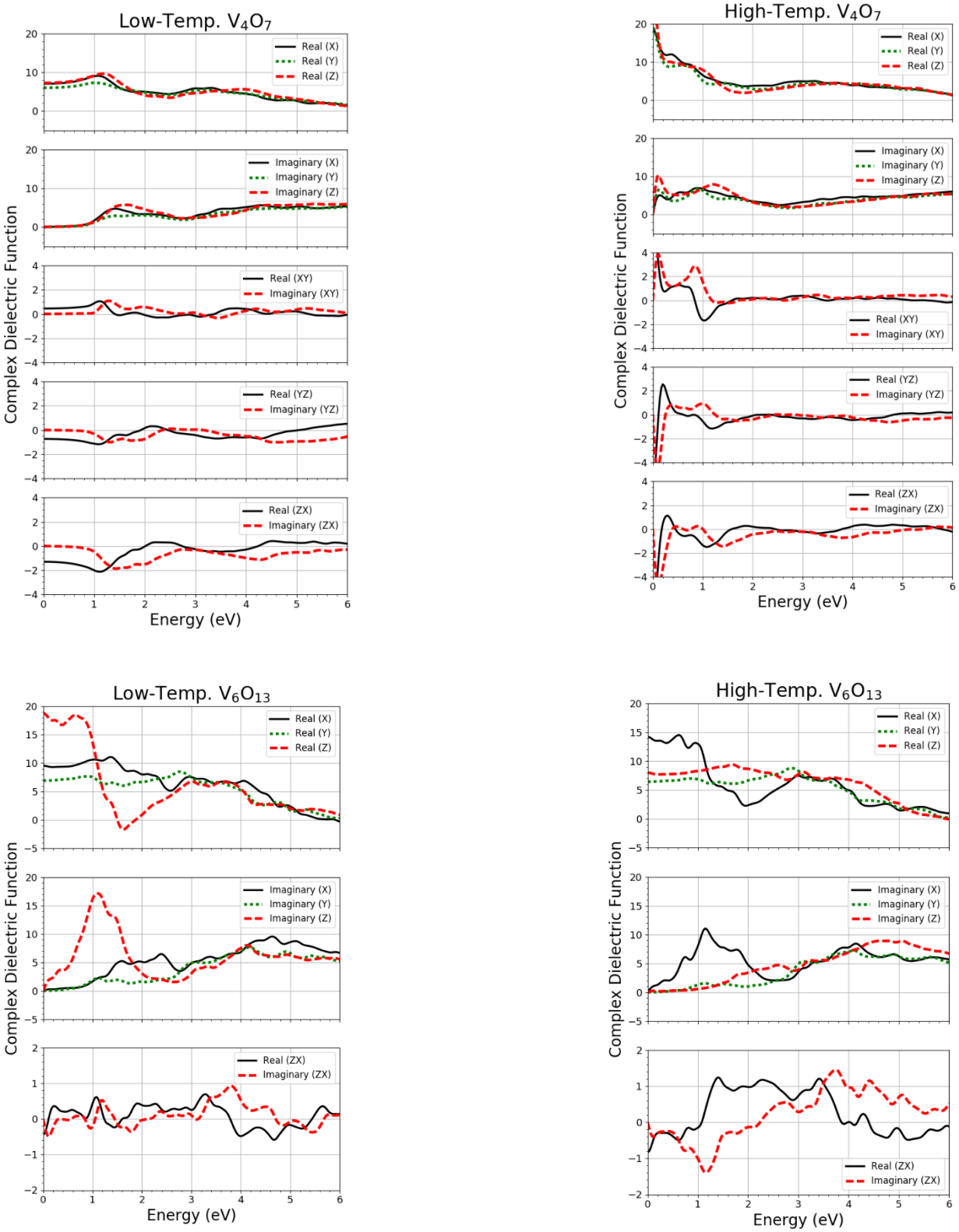

Figure S3: The real and imaginary parts of the complex dielectric function, as calculated through the GGA+U method, with a *U*-value of 3.25 eV. Due to the anisotropic nature of the materials, we have plotted the dielectric values in each direction according to the level of anisotropy within the compound. For monoclinic and triclinic compounds, the off-diagonal components are also shown.

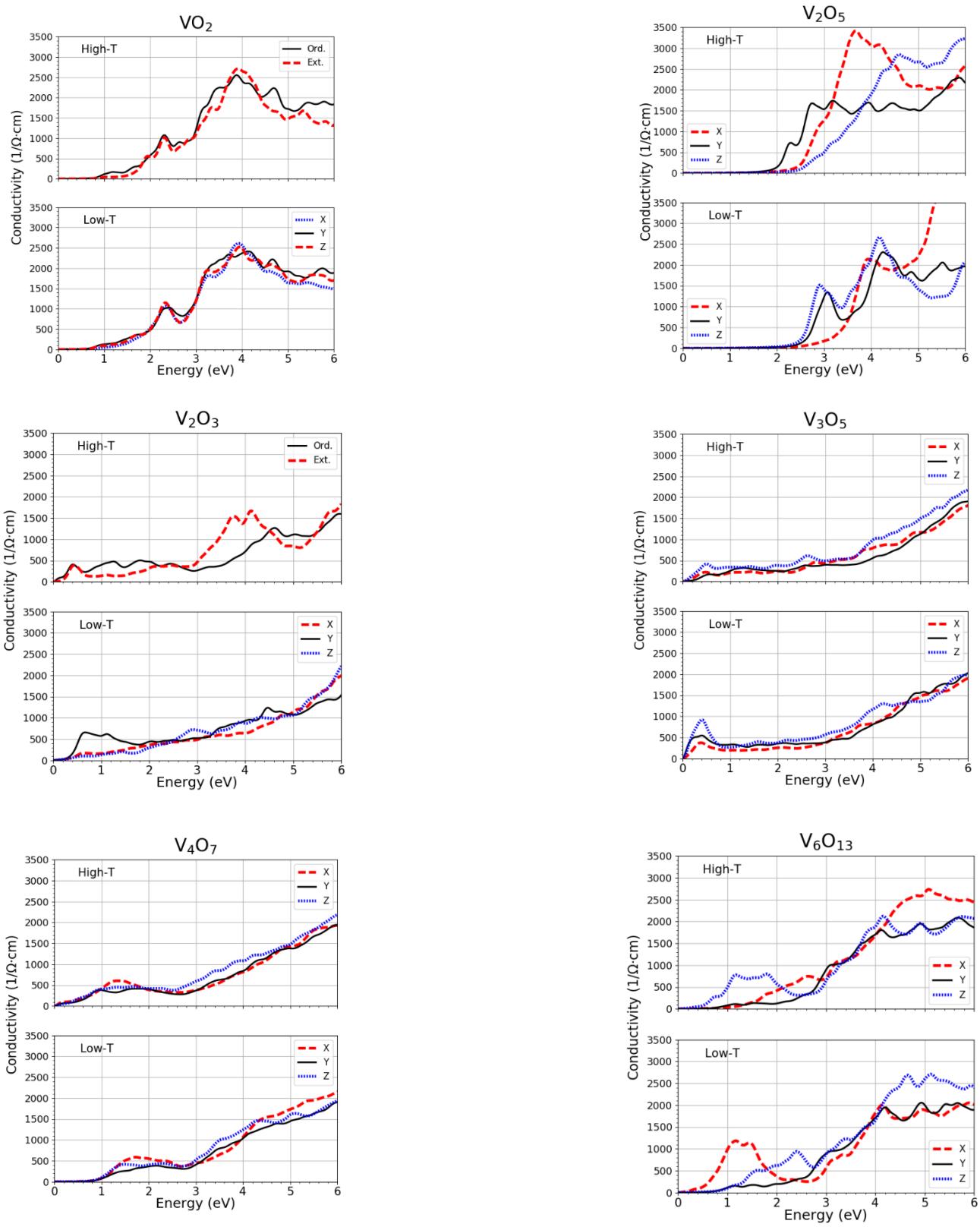

Figure S4: Optical conductivity of each compound, plotted as a function of photon energy, as found through the GGA+U method. Due to the anisotropic nature of the materials, we have plotted the values of the conductivity in each direction according to the level of anisotropy within the compound.