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ACCESSORY PUBLICATION

Synthesis, Structure and Theoretical Investigations of an Alkaline Earth Vanadate Oxide Compound ($Ca_4V_4O_{14}$): Electronic, Optical and Chemical Bond Properties

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Table S1. Selected bond lenghts (Å) and bond angles (°) for 1

V1-O1^{A}	2.053(3)	Ca1-O1^{A}	2.467(3)	Ca2-O2^{C}	2.938(3)
V1-O2	1.864(3)	Ca1-O1	3.289(3)	Ca2-O3^{E}	2.392(3)
V1-O2^{H}	1.883(3)	Ca1-O2	2.333(3)	Ca2-O3^{D}	2.413(3)
V1-O6	1.651(3)	Ca1-O3	3.453(3)	Ca2-O4	3.166(3)
V1-O7	1.672(3)	Ca1-O4	2.455(3)	Ca2-O5	2.423(3)
V2-O1	1.740(3)	Ca1-O4^{C}	2.407(3)	Ca2-O5^{G}	2.532(3)
V2-O3	1.695(3)	Ca1-O5^{B}	2.391(3)	Ca2-O6^{F}	2.406(3)
V2-O4	1.689(3)	Ca1-O6^{D}	2.462(3)	Ca2-O6	3.629(3)
V2-O5	1.730(3)	Ca1-O7^{A}	2.310(3)	Ca2-O7^{D}	2.317(3)
O6-V1-O7	112.40(14)	O2-V1-O1^{A}	80.56(12)	O4-V2-O5	106.90(15)
O6-V1-O2	117.46(13)	O2^{H}-V1-O1^{A}	158.43(12)	O3-V2-O5	109.12(14)
O7-V1-O2	129.98(14)	O2-V1-O2^{H}	80.13(13)	O4-V2-O1	108.37(14)

O6-V1-O2^{H}	101.58(14)	O6-V1-O1^{A}	95.79(13)	O3-V2-O1	112.09(14)
O7-V1-O2^{H}	94.09(13)	O4-V2-O3	109.60(14)	O5-V2-O1	110.62(14)
O7-V1-O1^{A}	90.97(13)				

Symmetry transformations used to generate equivalent atoms: ^{A} $-x + 2, -y + 1, -z + 1$; ^{B} $x, y - 1, z$; ^{C} $-x + 1, -y + 1, -z + 2$; ^{D} $x, y, z + 1$; ^{E} $-x + 1, -y + 2, -z + 2$; ^{F} $x, y + 1, z + 1$; ^{G} $-x + 2, -y + 2, -z + 2$; ^{H} $-x + 1, -y + 1, -z + 1$.

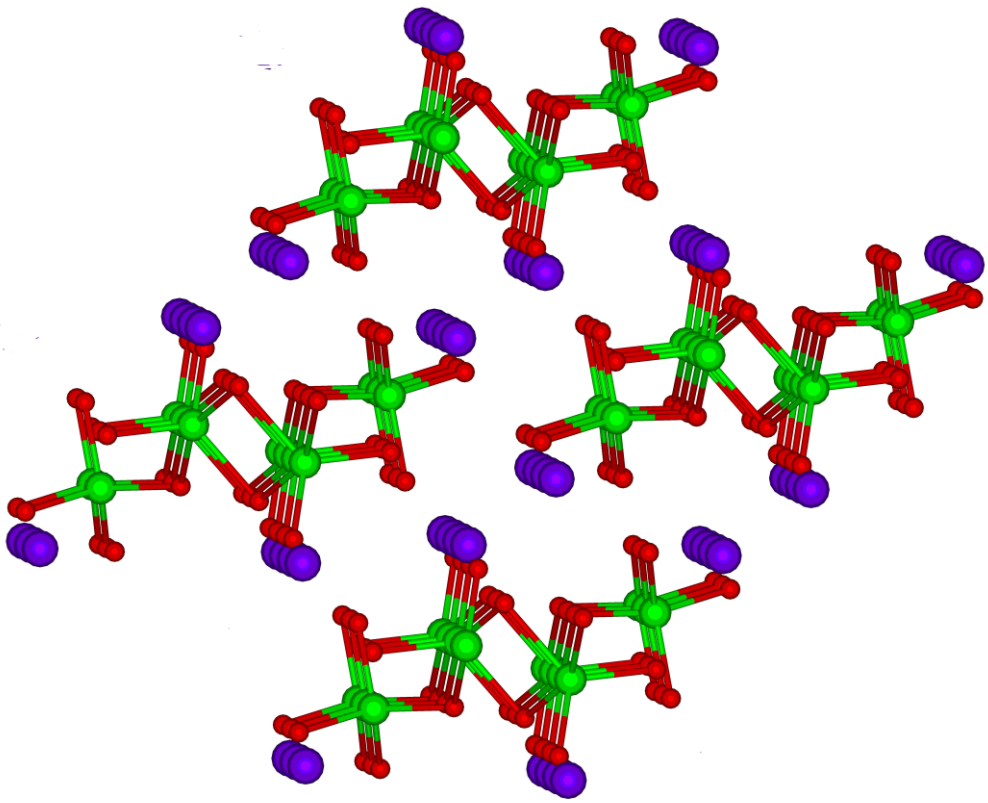

Fig. S1. Perspective view of the stacking structure in crystalline **1**. (Ca^{2+}: purple, V^{5+}: green, and O^{2-}: red)

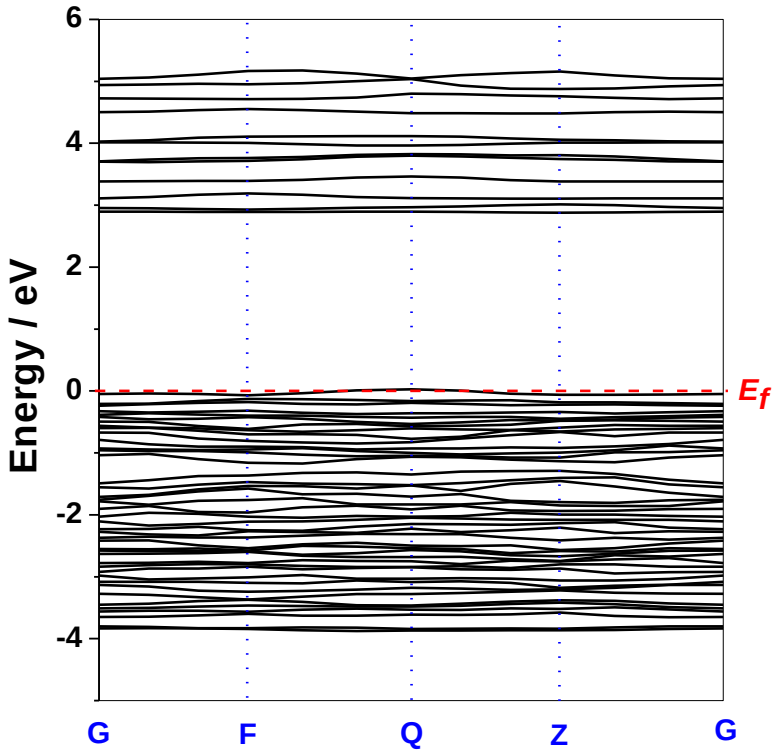

Fig. S2. Calculated energy band structure of **1**.

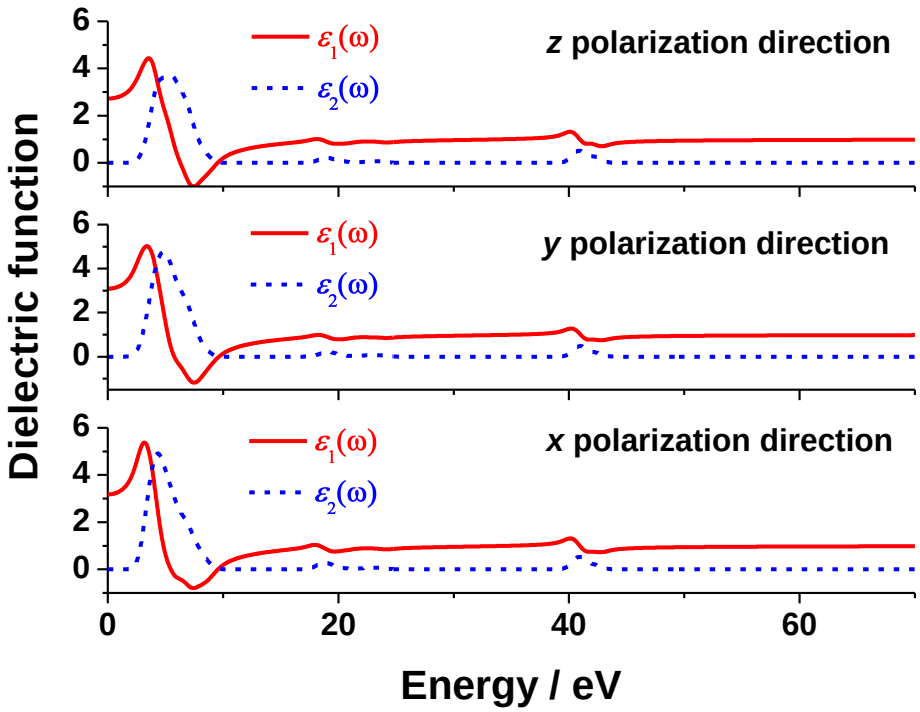

Fig. S3. Calculated dielectric function in different polarization directions of **1**.

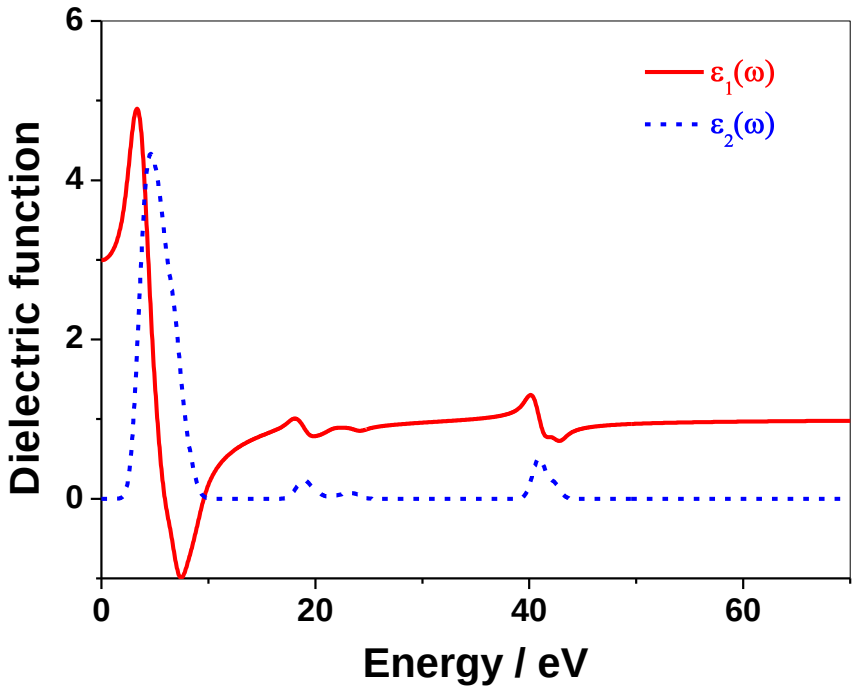

Fig. S4. Calculated real and imaginary part of dielectric functions of polycrystalline **1**.