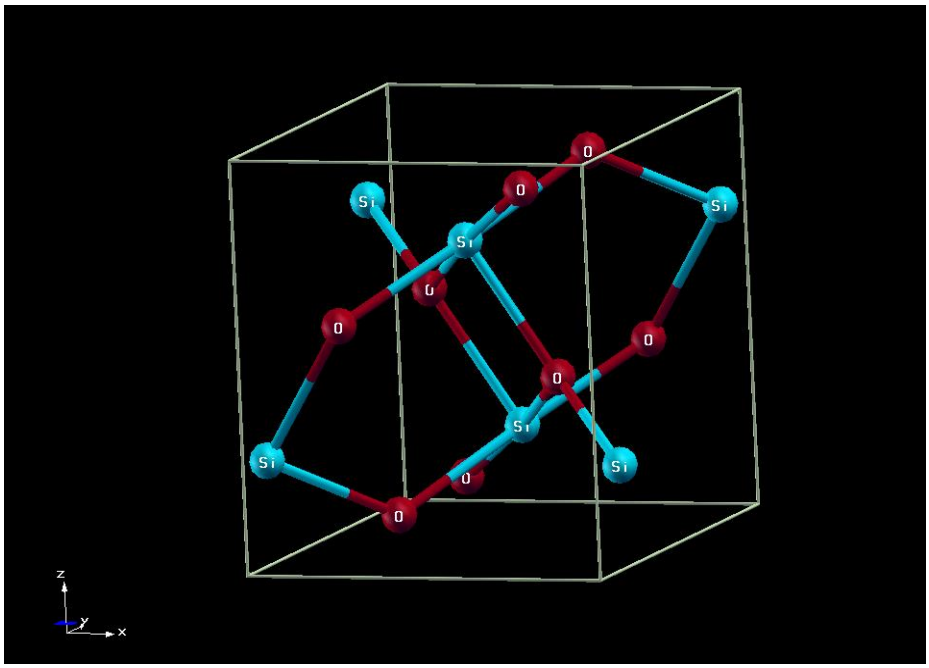

Figure A1-1 Unit cell of *seifertite.* Values of primitive translations **a**, **b**, **c** in the x, y, z directions and fractional coordinates of Si and O are given in the text. The coordination of Si by O is nearly octahedral and that of O by Si is trigonal.

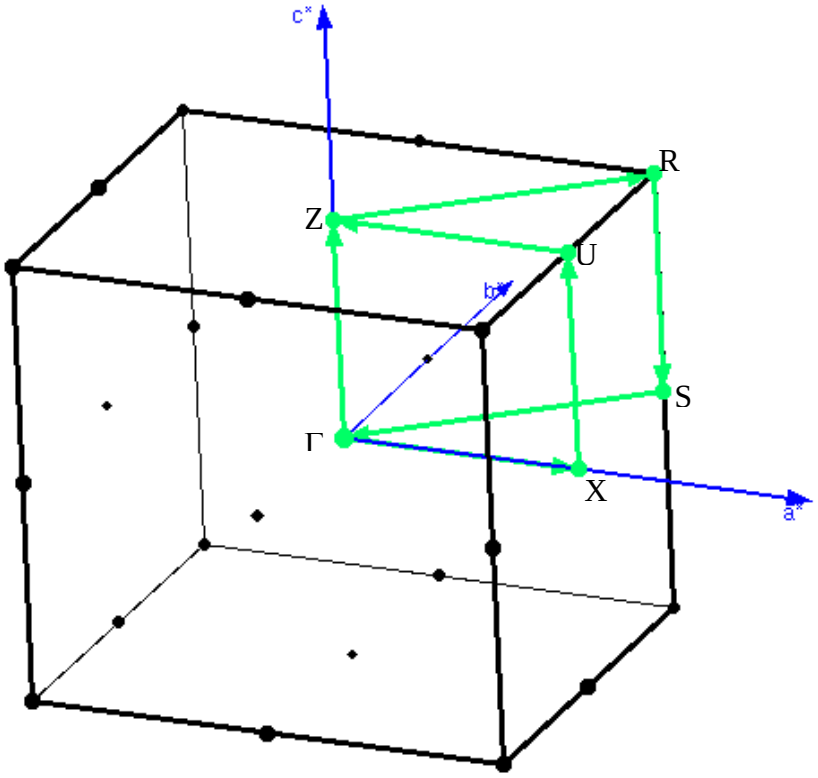

Figure A1-2 Brillouin zone of the orthorhombic lattice. Critical points chosen for the band structure representation are labeled as Γ (0,0,0), Z (0,0, ½), R (½, ½, ½), S (½, ½,0), X (½,0,0), U (½,0, ½). Lengths of the reciprocal vectors **a***, **b***, **c*** are in the ratio generated by the *seifertite* structure.

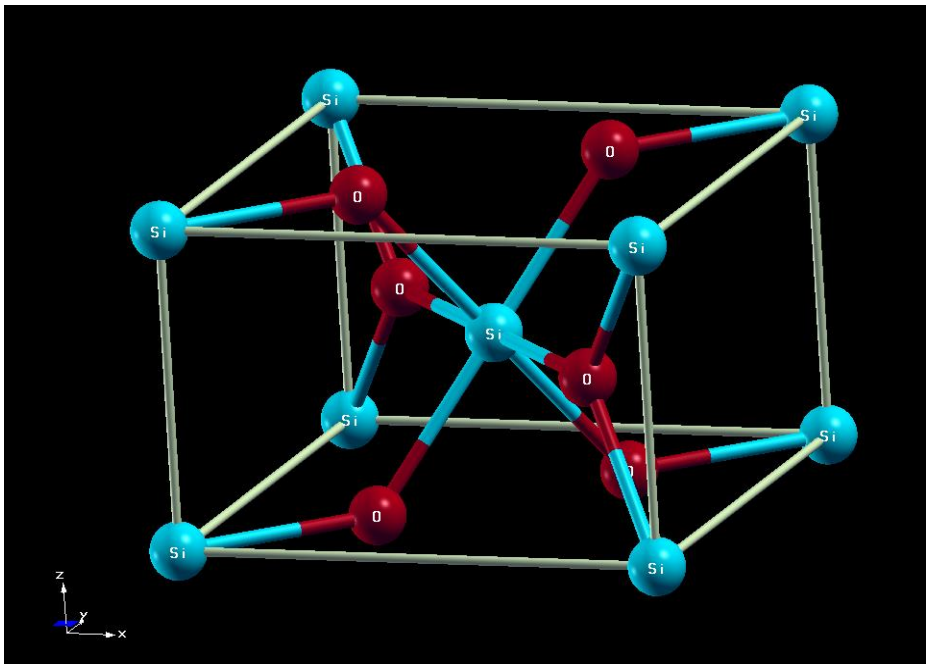

Figure A1-3 Unit cell of *stishovite*. Values of primitive translations **a**, **b**, **c** in the x, y, z directions and fractional coordinates of Si and O are given in the text. The coordination of Si by O is nearly octahedral and that of O by Si is trigonal.

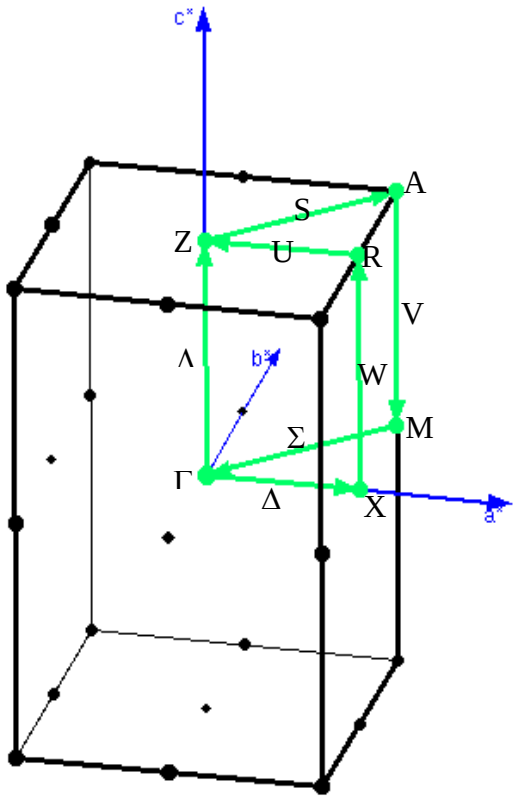

Figure A1-4 Brillouin zone of the tetragonal lattice. Critical points chosen for the band structure representation are labeled as Γ (0,0,0), Z (0,0, ½), A (½, ½, ½), M (½, ½,0), X (½,0,0), R (½,0, ½). Intermediate points Λ, S, V, Σ, Δ, W and U have coordinates specified in the klist_band for the tetragonal lattice. Lengths of the reciprocal vectors **a***, **b***, **c*** are in the ratio yielded by the *stishovite* structure.

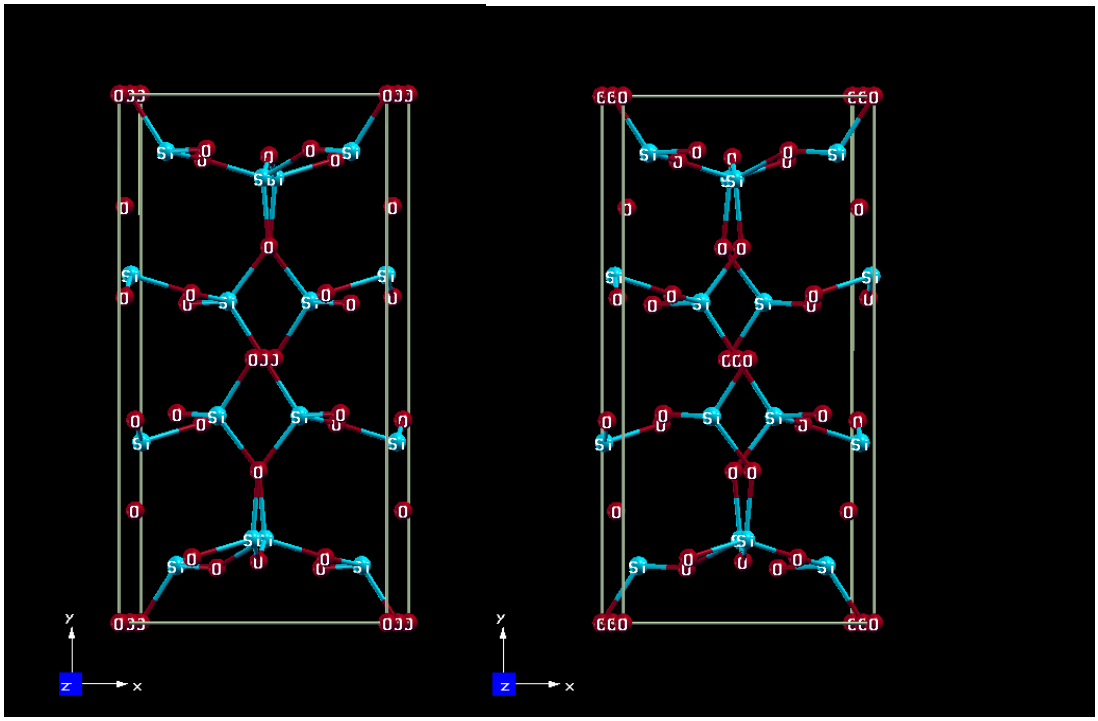

Figure A1-5 Unit cell of *coesite* as a stereo picture. Values of primitive translations **a**, **b**, **c** in the x, y, z directions and fractional coordinates of Si and O are given in the text. The coordination of Si by O is tetrahedral and that of O by Si is two-fold. O atoms at (0,0,0) and (1/2,1/2,1/2) are linearly coordinated to the nearest two Si neighbors, a feature that has influence on distribution of levels in the valence band.

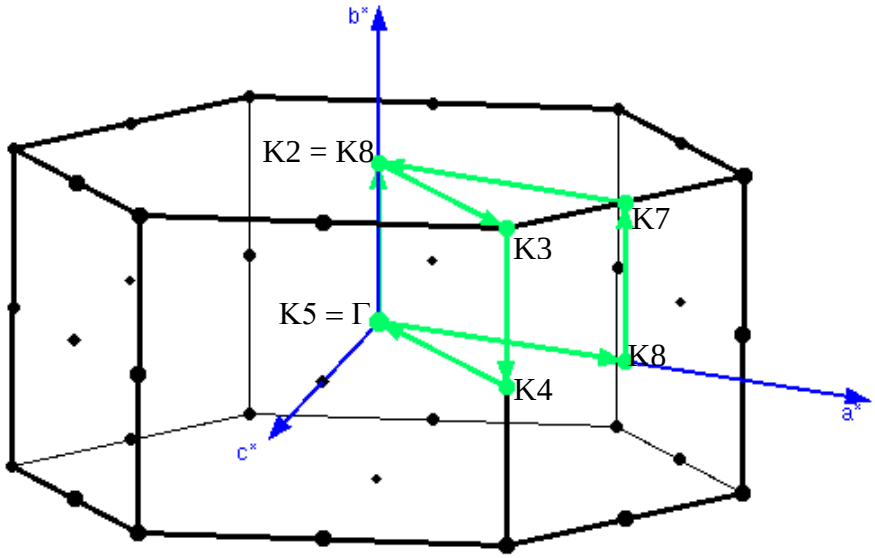

Figure A1-6 Brillouin zone of the monoclinic, nearly hexagonal lattice about the **b*** axis. Critical points chosen for the band structure representation are labeled as:
Γ (0,0,0), K2 (0, ½, 0), K3 (0.335, ½, 0.33), K4 (0.335,0, 0.33), K5 = Γ, K6 (½,0,0), K7 (½,½,0), K8 = K2.
The corresponding labels for the idealized hexagonal lattice are:
Γ ≡ [K1 = K5], A ≡ [K2 = K8], H ≡ K3, K ≡ K4, M ≡ K6 and L ≡ K7.
The lengths of and angles between the reciprocal vectors **a***, **b***, **c*** are in the ratio created by the *coesite* structure.

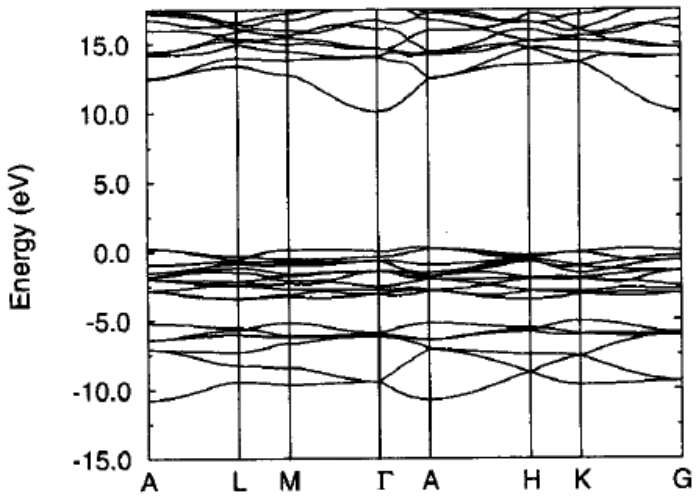

Figure A2-1. Calculated quasiparticle band structure of *α-quartz* in the GW approximation.

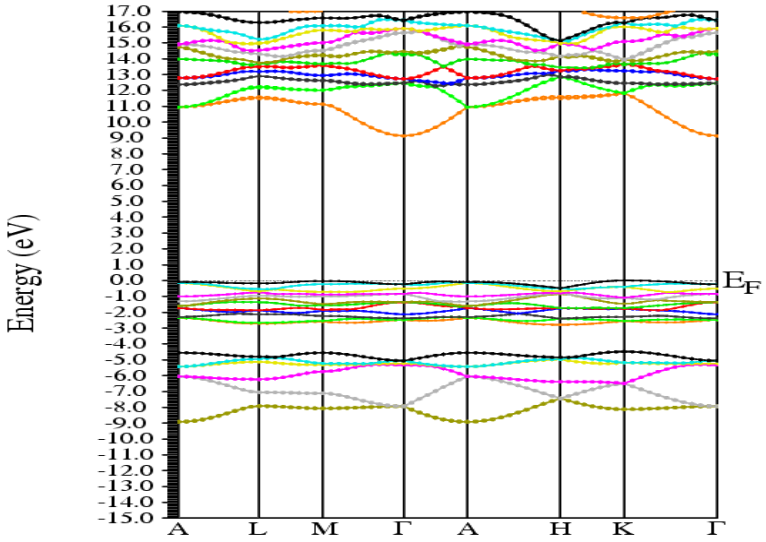

Figure A2-2. Calculated band structure of *α-quartz* in the mBJ/spin-polarized/Si3d-SIC approximation.

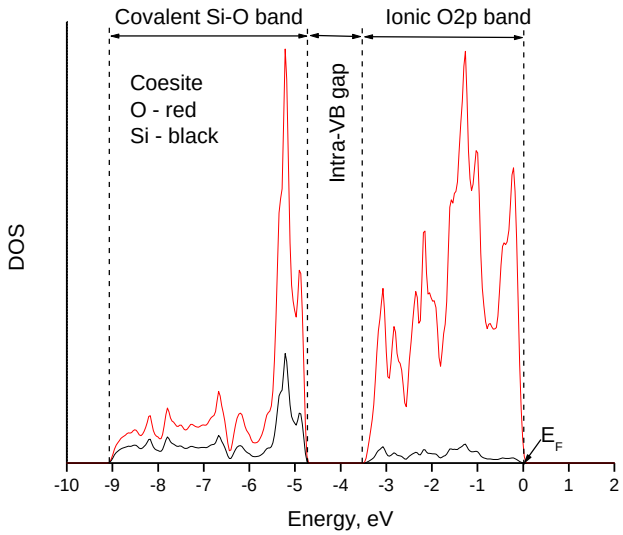

Figure A3-1. Partial VB DOS of Si and O contributions in *coesite*, showing a separation of ionic O2p band from covalent Si-O band across a 1.3 eV intrinsic gap.

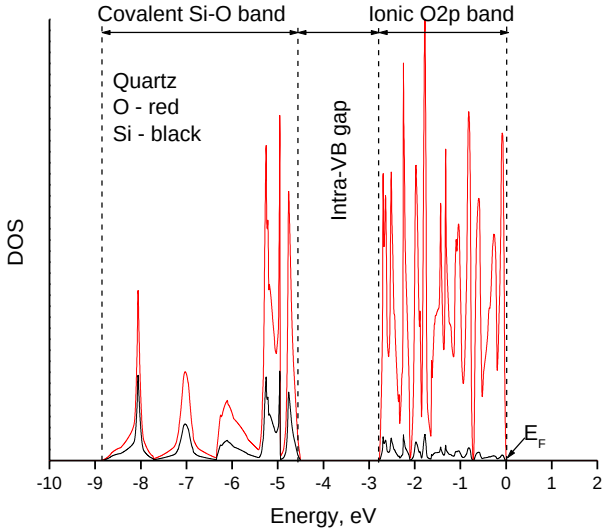

Figure A3-2. Partial VB DOS of Si and O contributions in *α-quartz*, showing a separation of ionic O2p band from covalent Si-O band across a 1.7 eV intrinsic gap. Common features of the two tetrahedral polymorphs *coesite* and *α-quartz* are: (a) low contributions of Si to the split-off upper portion of VB; (b) significant contributions of Si to the split-off lower portion of VB; and (c) overlap of Si and O contributions in the lower VB indicating covalent Si-O bonding.

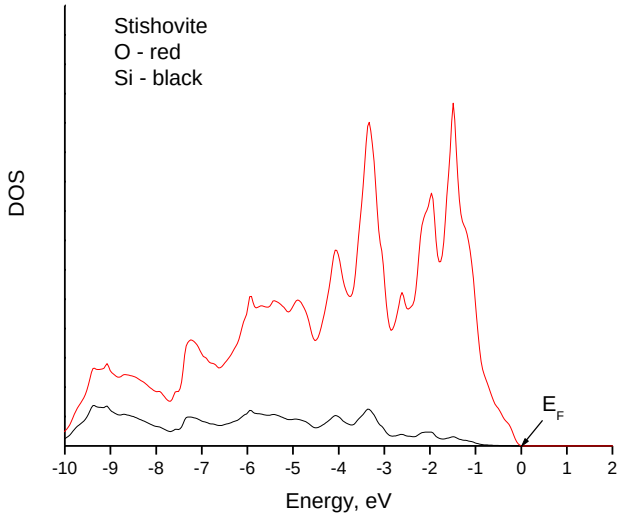

Figure A3-3. Partial VB DOS of Si and O contributions in *stishovite*, showing a continuous band dominated by O2p orbitals with small contribution of Si orbitals decreasing from the bottom to the top of VB.

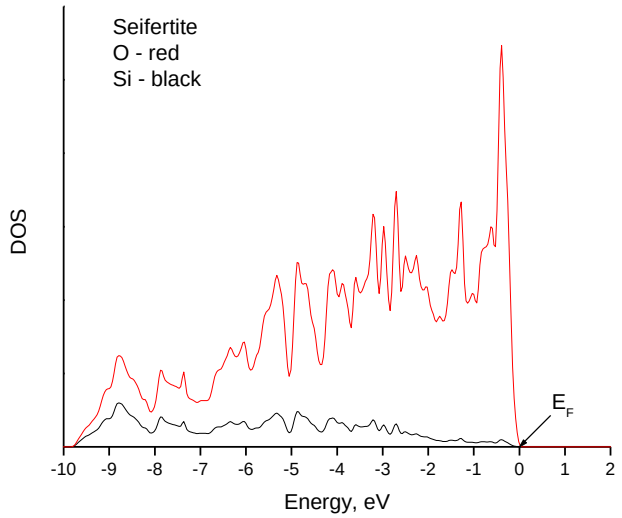

Figure A3-4. Partial VB DOS of Si and O contributions in *seifertite*, showing features similar to those of the *stishovite* VB in Figure A3-3.
Common features of the two octahedral polymorphs *stishovite* and *seifertite* entail continuous, predominantly O2p valence bands with small, progressively decreasing contributions of Si from the bottom to the top of the VB.