Supplementary data

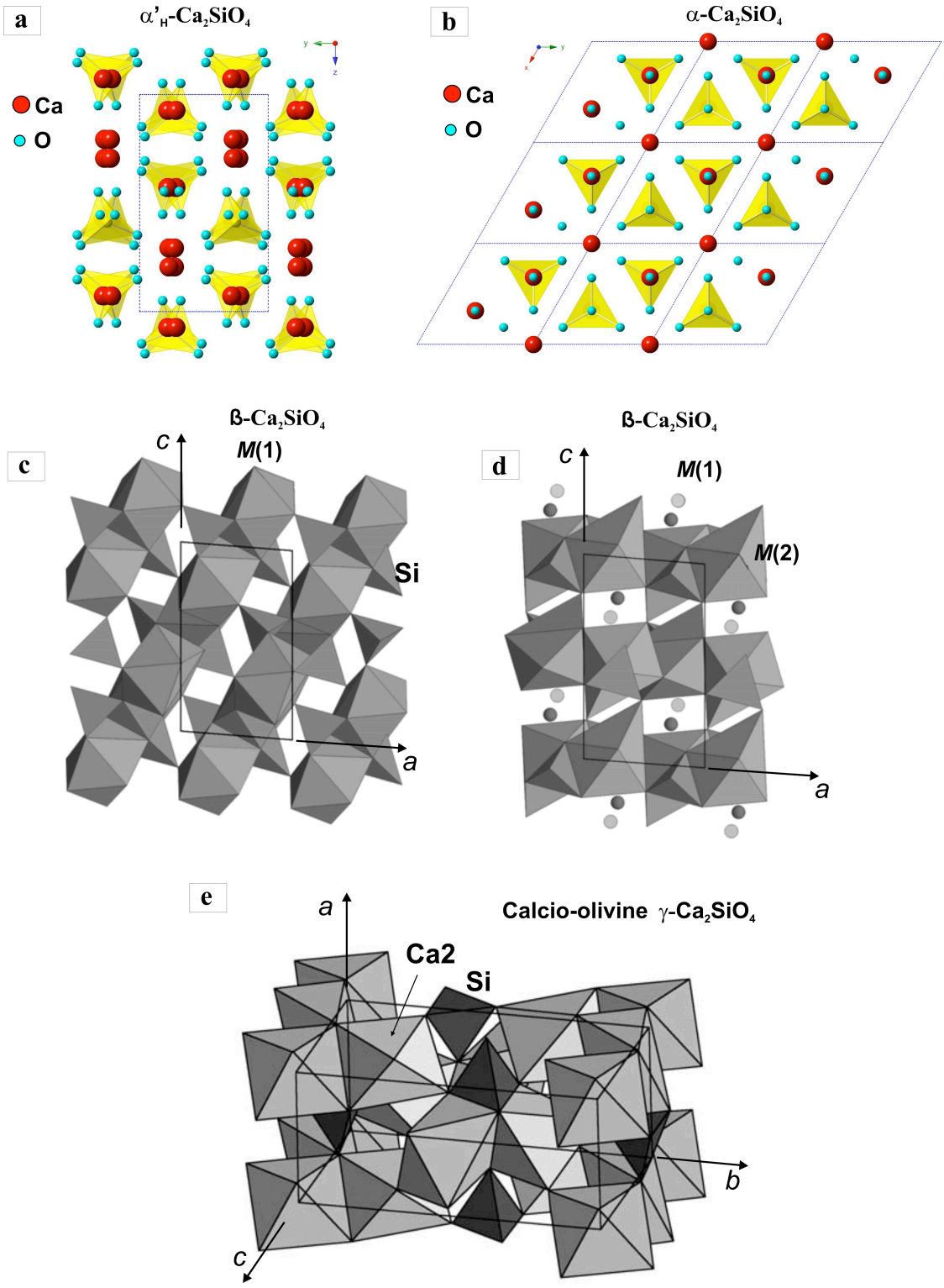

Figure S1. Polyhedral representation of the structures of Ca_2SiO_4 polymorphic modifications: α'_H - Ca_2SiO_4 (**a**), α - Ca_2SiO_4 (**b**), β-Ca_2SiO_4 (larnite) (**c, d**), and γ - Ca_2SiO_4 (calcio-olivine) (**e**).

(**a, b**) Rietveld crystal structure refinements of (for ?) α'_H - Ca_2SiO_4 (**a**) and α - Ca_2SiO_4 (**b**) are shown in comparable views (modified after Mumme et al. 1995); Si within yellow tetrahedra.

(**c, d**) Larnite (β-Ca_2SiO_4) structure in projections on the (010) plane: **(c)** layers of *M*(1) eight-vertex Ca polyhedra and **(d)** framework of *M*(2) seven-vertex Ca polyhedra. Ca atoms in the *M*(1) position at the levels $y \sim 0$ and 0.5 are indicated by lighter and darker circles, respectively (Yamnova et al. 2011).
(e) Polyhedral representation of the structure of calcio-olivine (γ-Ca_2SiO_4) (Gobechiya et al. 2008).

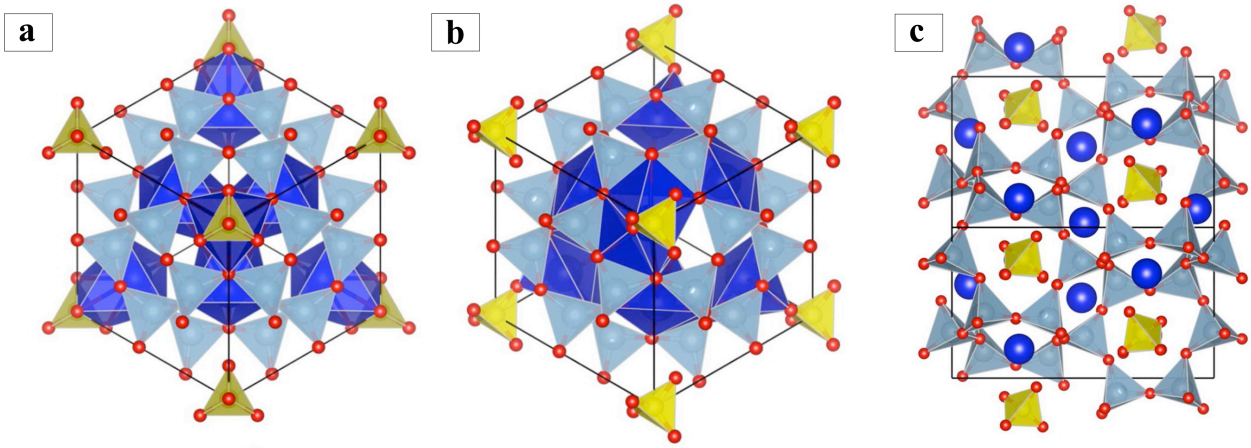

Figure S2. Calculated crystal structures of $Ca_4Al_6O_{12}(SO_4)$ polymorphic modifications: **(a)** cubic (*I*$\underline{4}$3*m*) – ye'elimite, **(b)** tetragonal (*I*$\underline{4}$) phase, and **(c)** orthorhombic (*Pcc*2) phase.

Ca denoted within dark-blue prisms, Al within light-blue tetrahedra, S within yellow tetrahedra, and O are red. CaO bonds are omitted in **(c)** after (Cuesta et al. 2013).

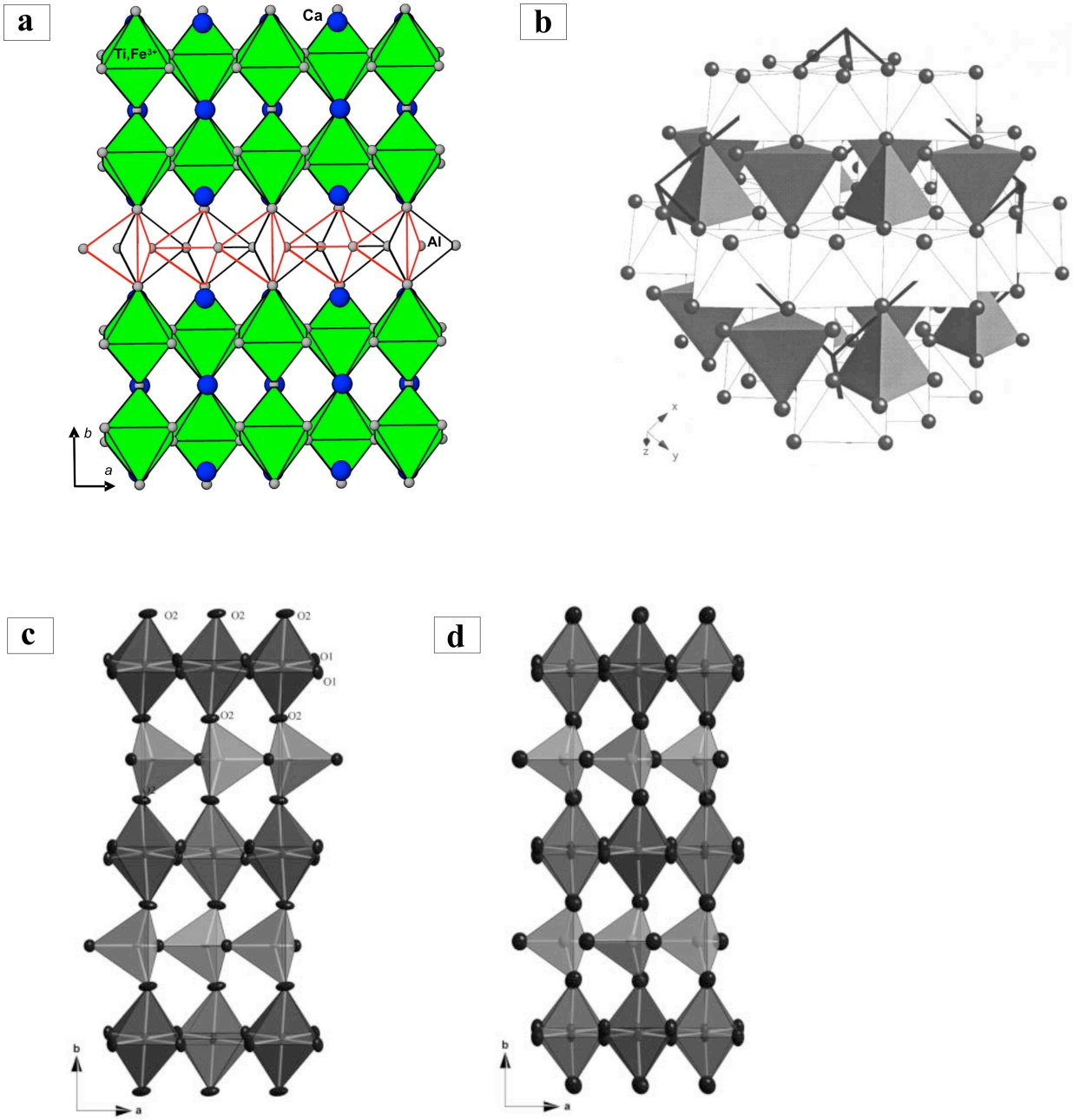

Figure S3. Structure plots of main opaque minerals of YL rocks and cement clinkers.

(a) Structural topology in a projection along ***c*** axis for shulamitite, $Ca_3TiFe^{3+}AlO_8$ showing the overlay of two orientations of chains of Al-dominant tetrahedra extending along the ***a*** axis (Sharygin et al. 2013).
(b) Structure plot of magnesioferrite, $MgFe_2O_4$ (at T = 28°C). The tetrahedral and octahedral cation sites are shown in grey and white, respectively, and the O atoms as small circles (Antao et al. 2005).
(c, d) Comparison of the structural topology in a projection along ***c*** axis for srebrodolskite, $Ca_2Fe_2O_5$ with *Pnma* symmetry **(c)** and Al-rich brownmillerite $Ca_2Fe_{0.64}Al_{1.36}O_6$ with *I2mb* symmetry **(d)** displaying the different stacking sequences of the tetrahedral chains (Redhammer et al. 2004).

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