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Supplementary material: Structure from glass to melt: a case study along the $MgSiO_3$–$CaSiO_3$ join using neutron and X-ray diffraction

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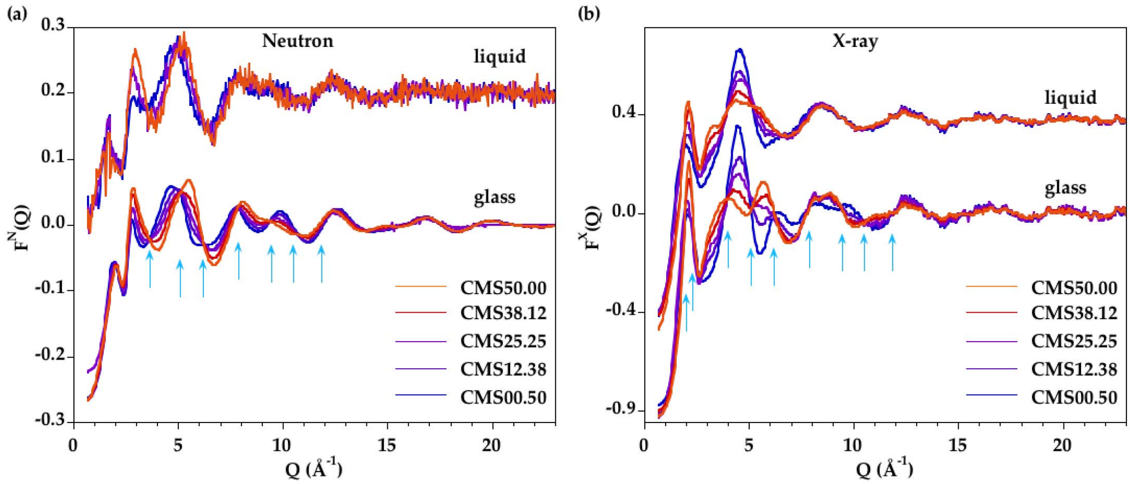
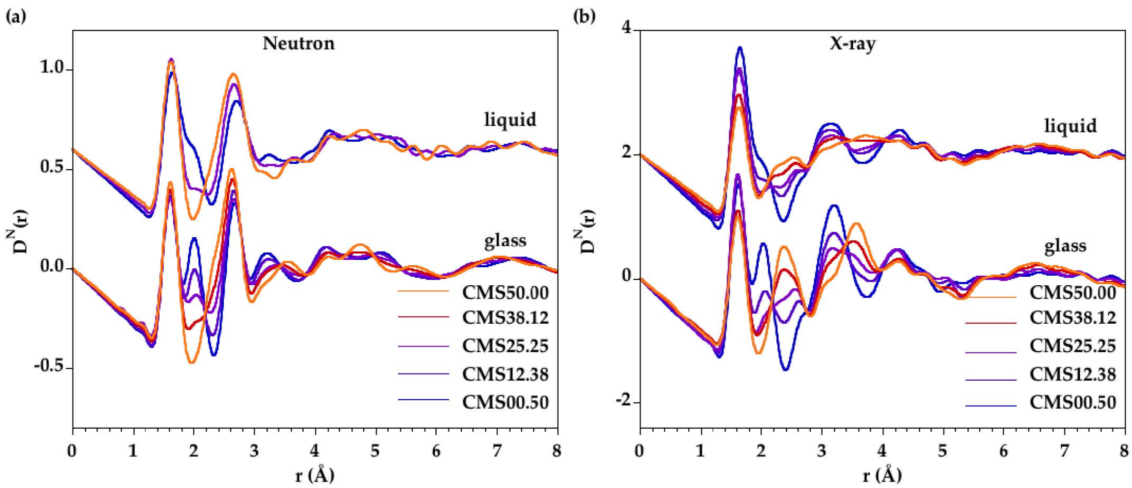
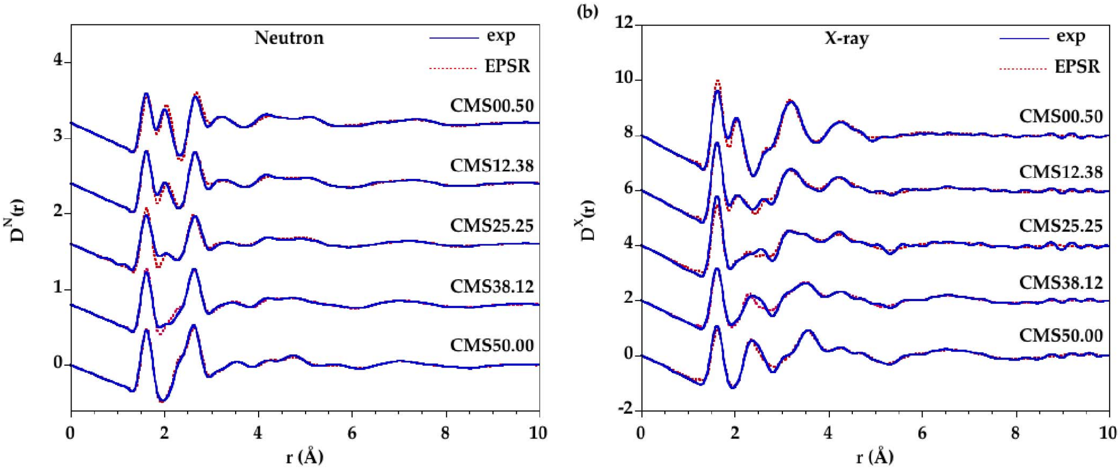


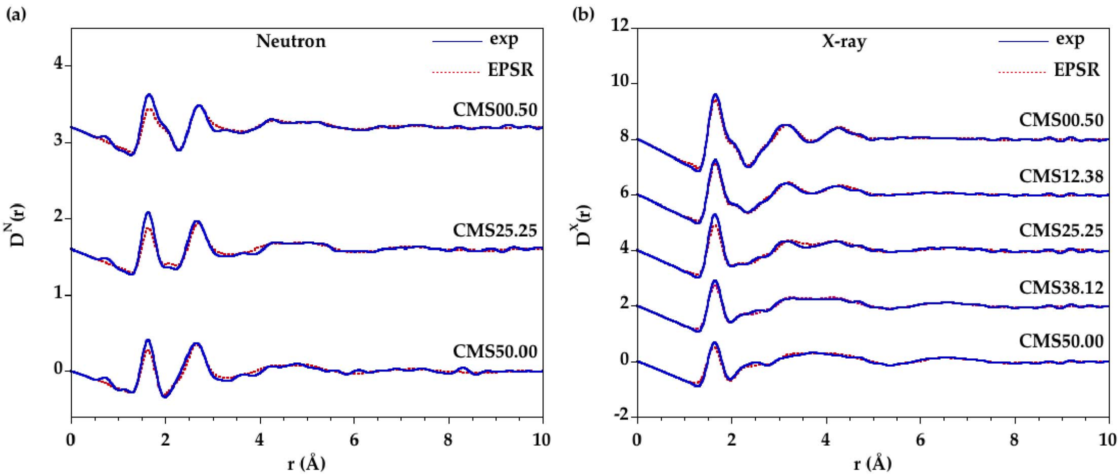
Supplementary Figure S1. Experimental structure factors for the CMS glasses/liquids series for (a) neutron diffraction and (b) X-ray diffraction. The isobestic points are indicated as vertical solid arrows.



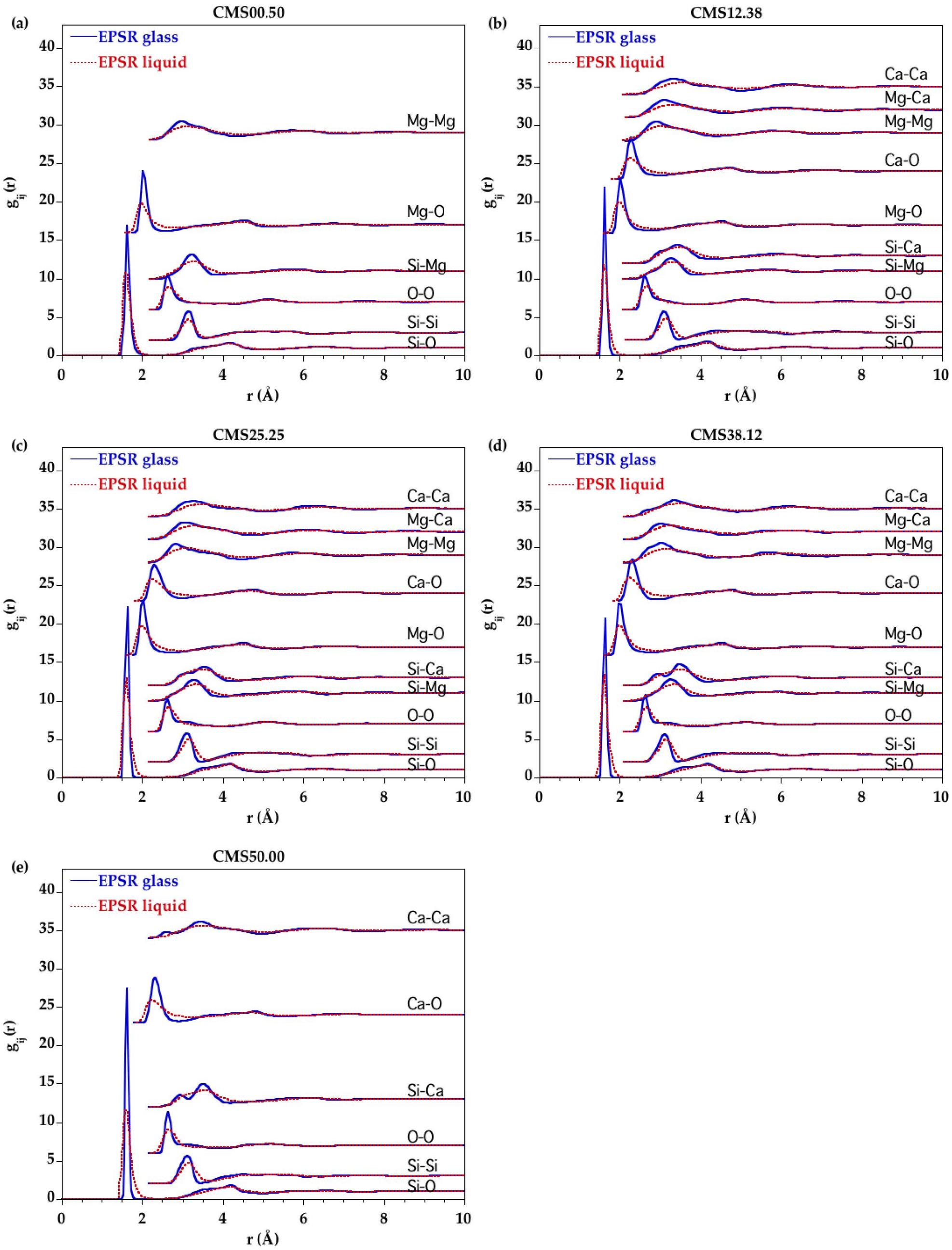
Supplementary Figure S2. Pair distribution functions for the CMS glasses/liquids series for (a) neutron diffraction and (b) X-ray diffraction.



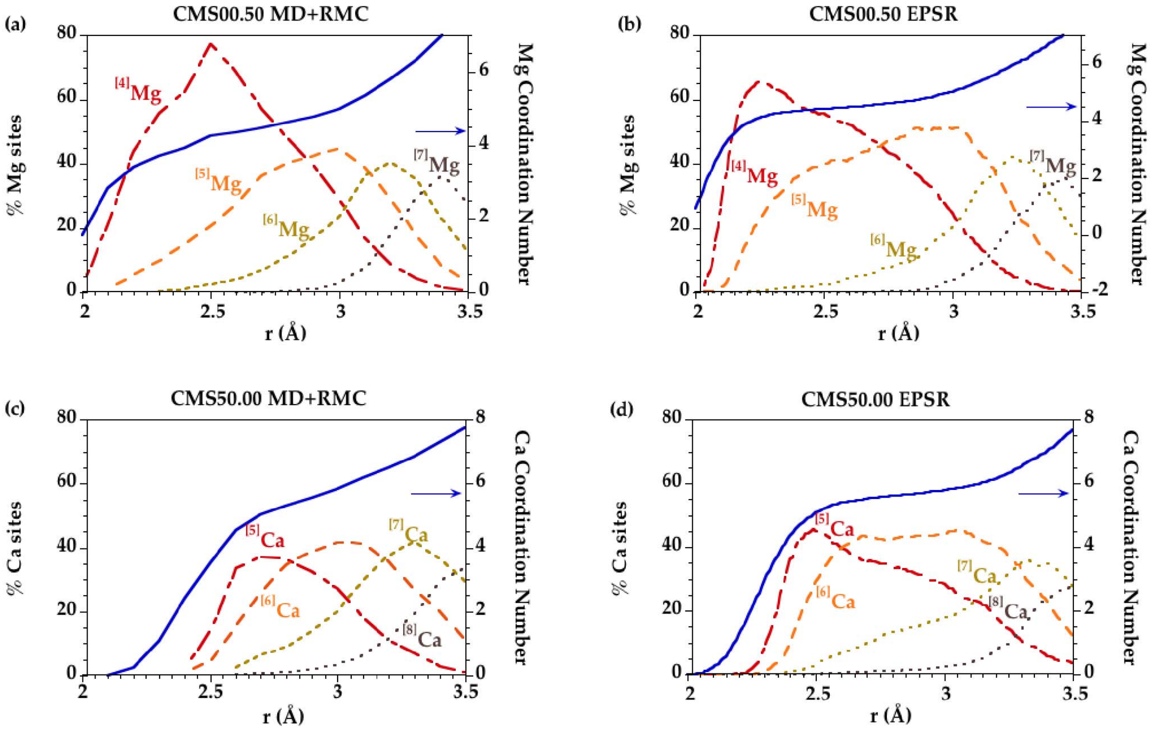
Supplementary Figure S3. Comparison of the pair distribution function obtained experimentally (blue solid curve) and by EPSR modeling (red dashed curve) for the CMS glasses. (a) Neutron diffraction and (b) X-ray diffraction. Fourier transform were obtained from the structure factors in Figure S3 with a Lorch modification function and using the range $0.56\ \text{Å}^{-1} \leq Q \leq 22\ \text{Å}^{-1}$.



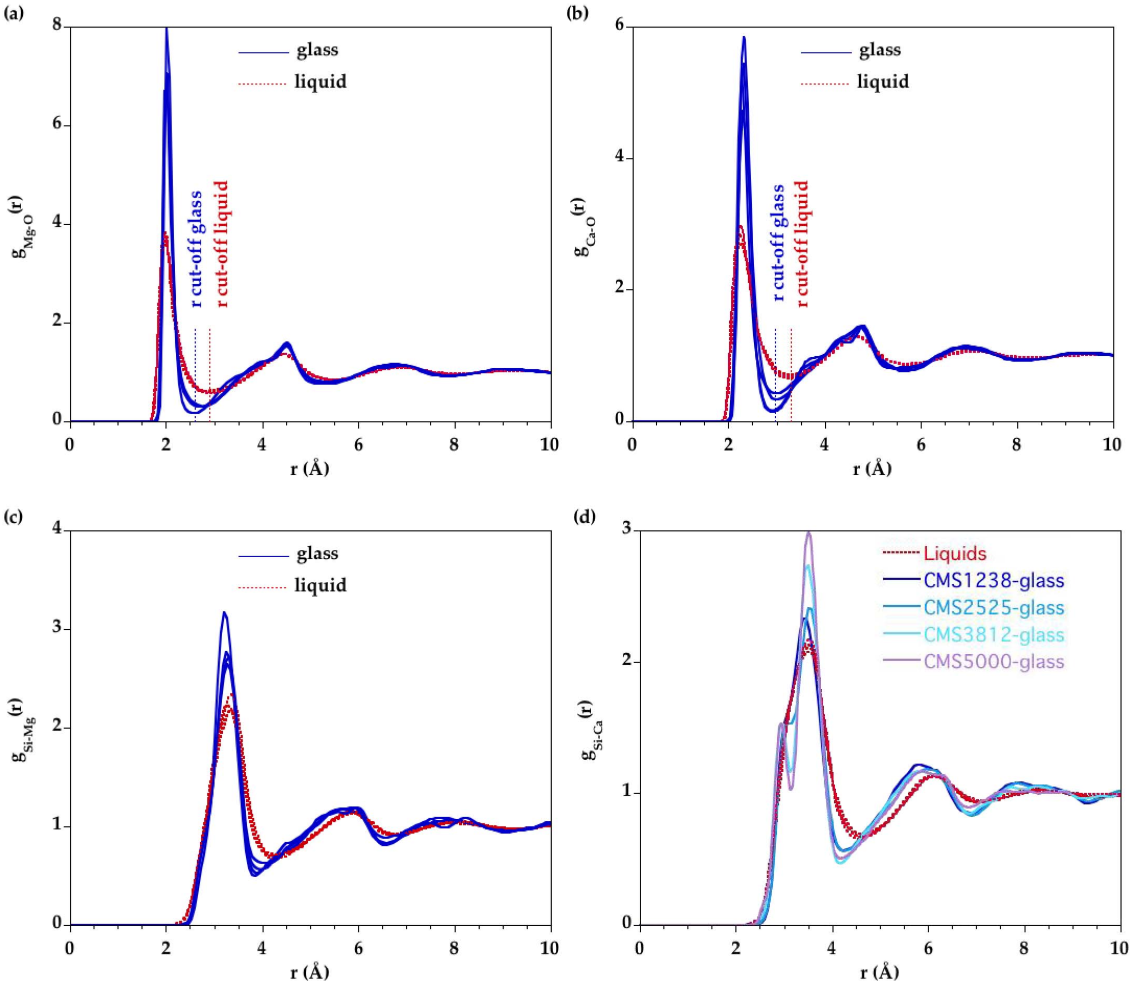
Supplementary Figure S4. Comparison of the pair distribution function obtained experimentally (blue solid curve) and by EPSR modeling (red dashed curve) for the CMS liquids. (a) Neutron diffraction and (b) X-ray diffraction. Fourier transform were obtained from the structure factors in Figure S4 with a Lorch modification function and using the range $0.56\ \text{Å}^{-1} \leq Q \leq 22\ \text{Å}^{-1}$.



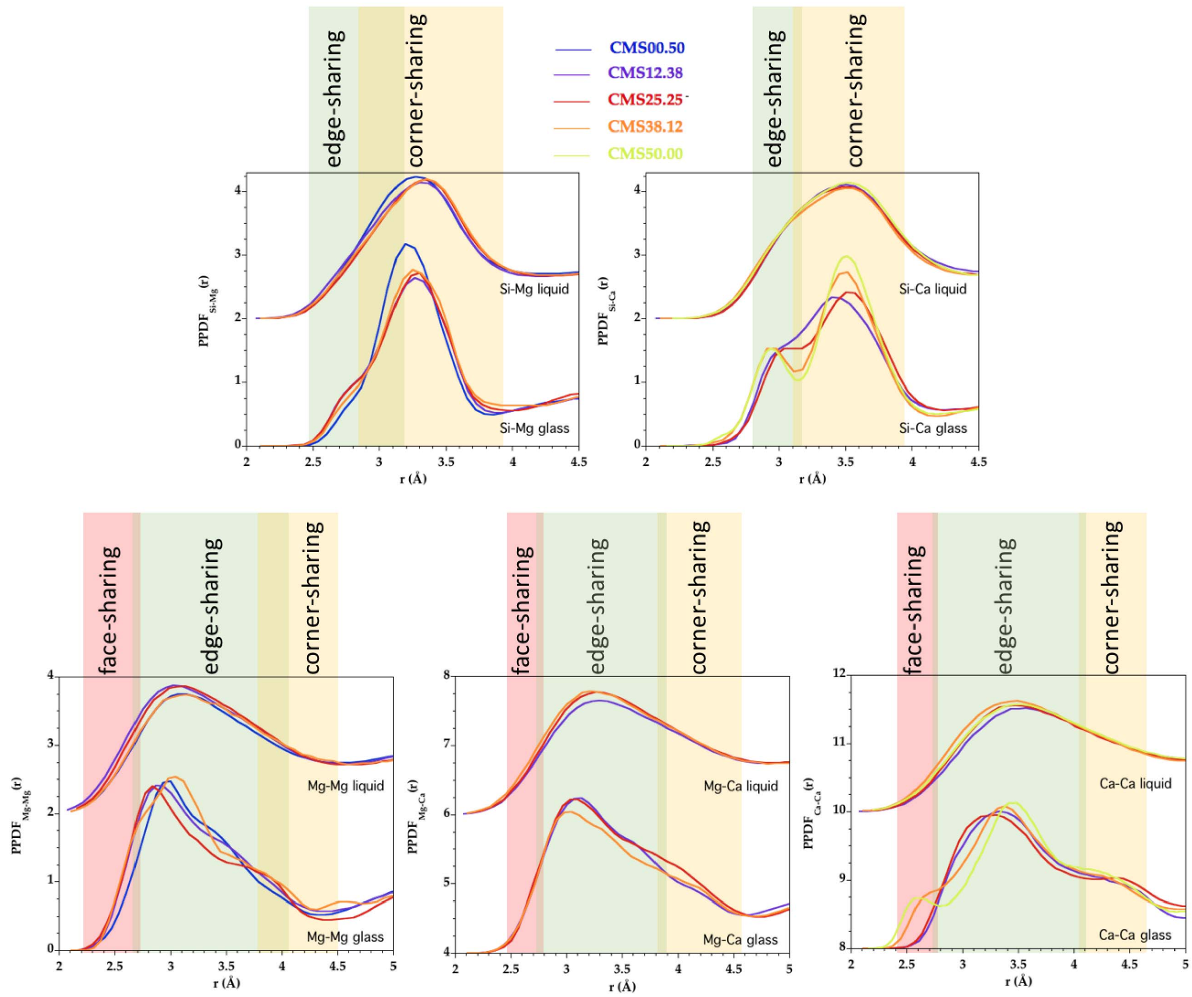
Supplementary Figure S5. Comparison of the EPSR partial distribution functions for the glass (blue curve) and the liquid (red dashed curve) corresponding to the samples (a) CMS00.50, (b) CMS12.38, (c) CMS25.25, (d) CMS38.12 and (e) CMS50.00.



Supplementary Figure S6. Evolution as a function of the cutoff distance of the average coordination number (right axis) and of the cation site distribution (left axis). Results for Mg in CMS00.50 glass are calculated from (a) the MD+RMC model from Cormier and Cuello [Cormier and Cuello, 2012] and from (b) the EPSR model in the present paper. Results for Ca in CMS50.00 glass are calculated from (c) the MD+RMC model from Cormier and Cuello [Cormier and Cuello, 2012] and from (d) the EPSR model in the present paper.



Supplementary Figure S7. EPSR partial distribution functions highlighting the differences between the CMS glasses and liquids for (a) the Mg–O pair, (b) the Ca–O pair, (c) the Si–Mg pair and (d) the Si–Ca pair.



Supplementary Figure S8. EPSR partial distribution functions for the CMS glasses/liquids, highlighting the bond length regions characteristics of face-, edge- and corner-sharing for (a) Si–Mg, (b) Si–Ca, (c) Mg–Mg, (d) Mg–Ca and (e) Ca–Ca pairs.

Reference

Cormier, L. and Cuello, G. J. (2012). Structural investigation of glasses along the $MgSiO_3$–$CaSiO_3$ join: diffraction studies. *Geochim. Cosmochim. Acta*, 122, 498–510.