

Local Structure and Magnetism of Fe₂O₃ Maghemite Nanocrystals: The Role of Crystal Dimension

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Molecular dynamics:

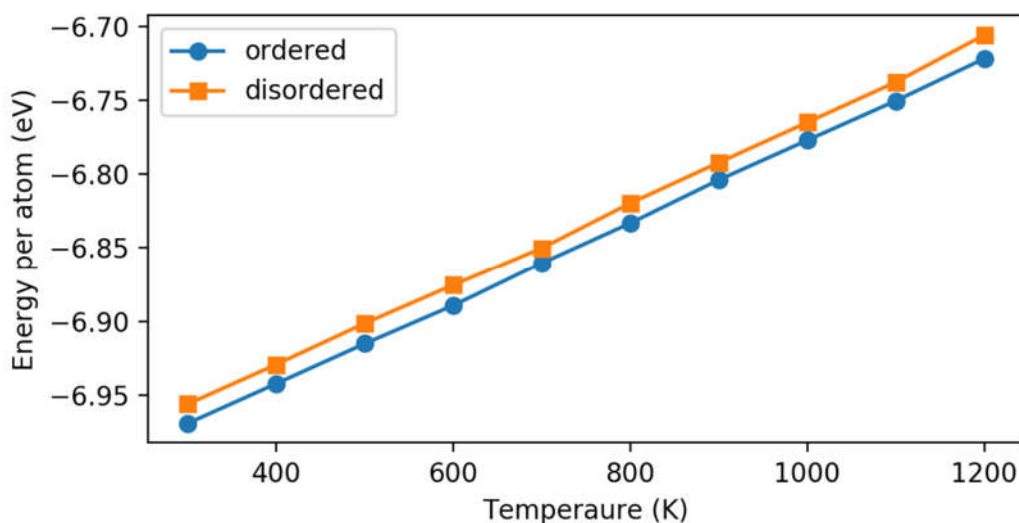


Figure S1. Calculated average internal energy as function of temperature for bulk ordered and disordered maghemite.

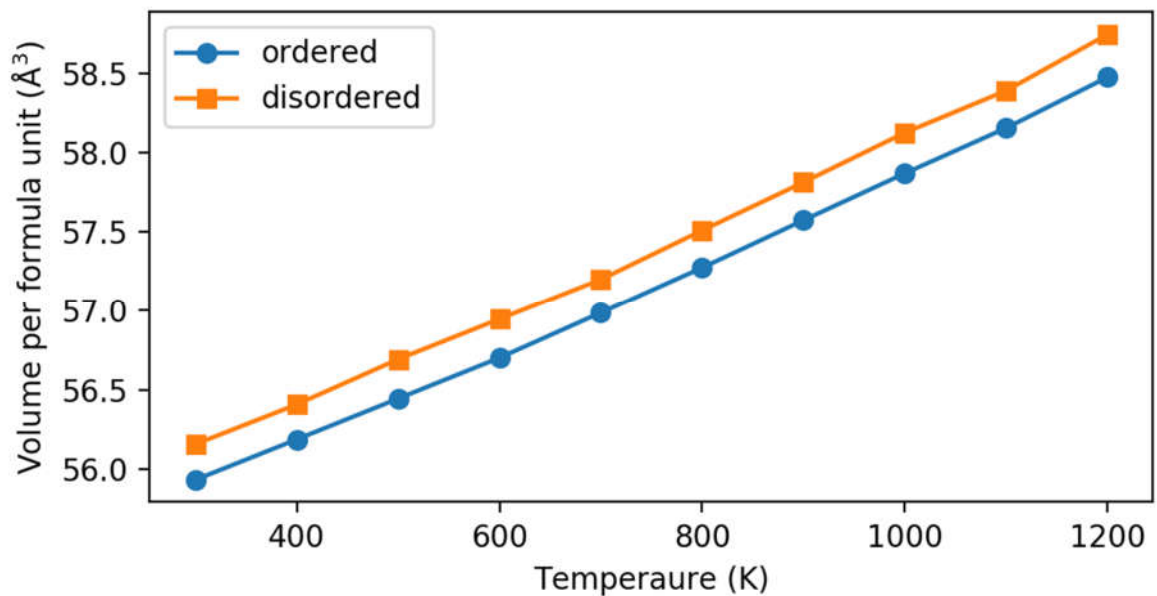


Figure S2. Calculated average volume per Fe_2O_3 as function of temperature for bulk ordered and disordered maghemite.

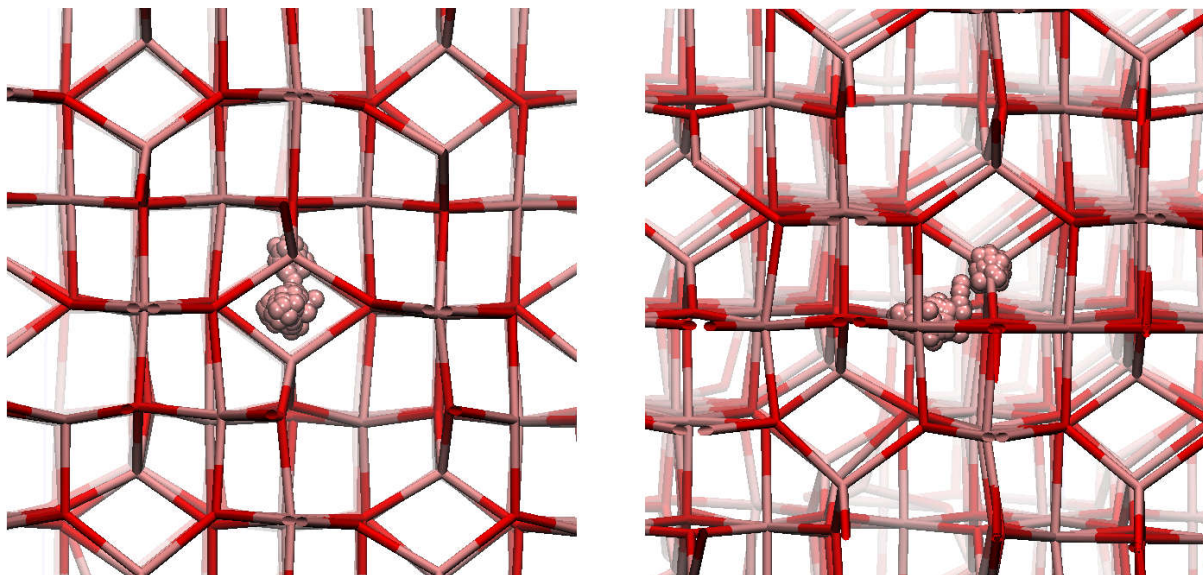


Figure S3. Molecular dynamics snapshots of the migration of an iron atom from a tetrahedral site to an octahedral site, at 1000 K. Left: view along the $[110]$. Right: view along the $[010]$ direction. Iron ions are pale red in color; oxygen ions are dark red.

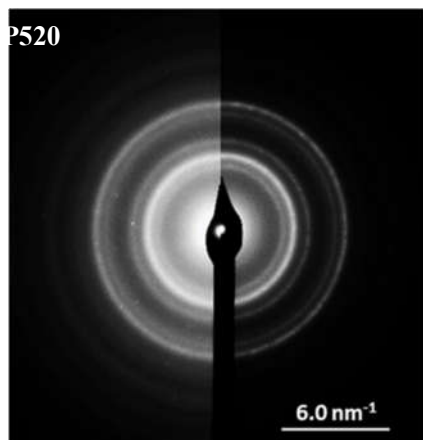


Figure S4. Electron diffraction for both microwave plasma synthesized samples.

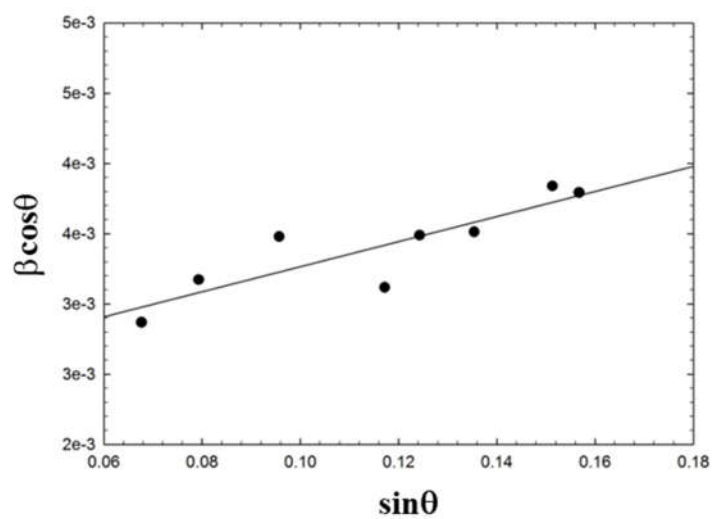


Figure S5. Example of Williamson Hall plot for sample P520.

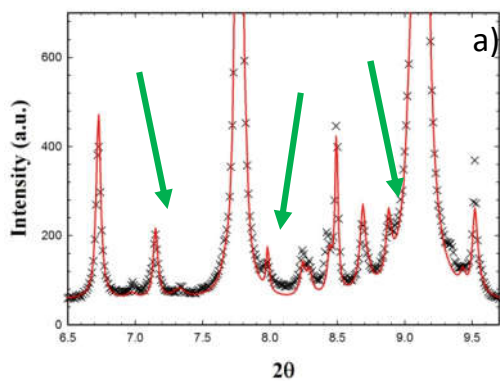


Figure S6. 2theta range from 6 to 10 of the Aldrich sample. The superstructure peak are highlighted by the arrows.

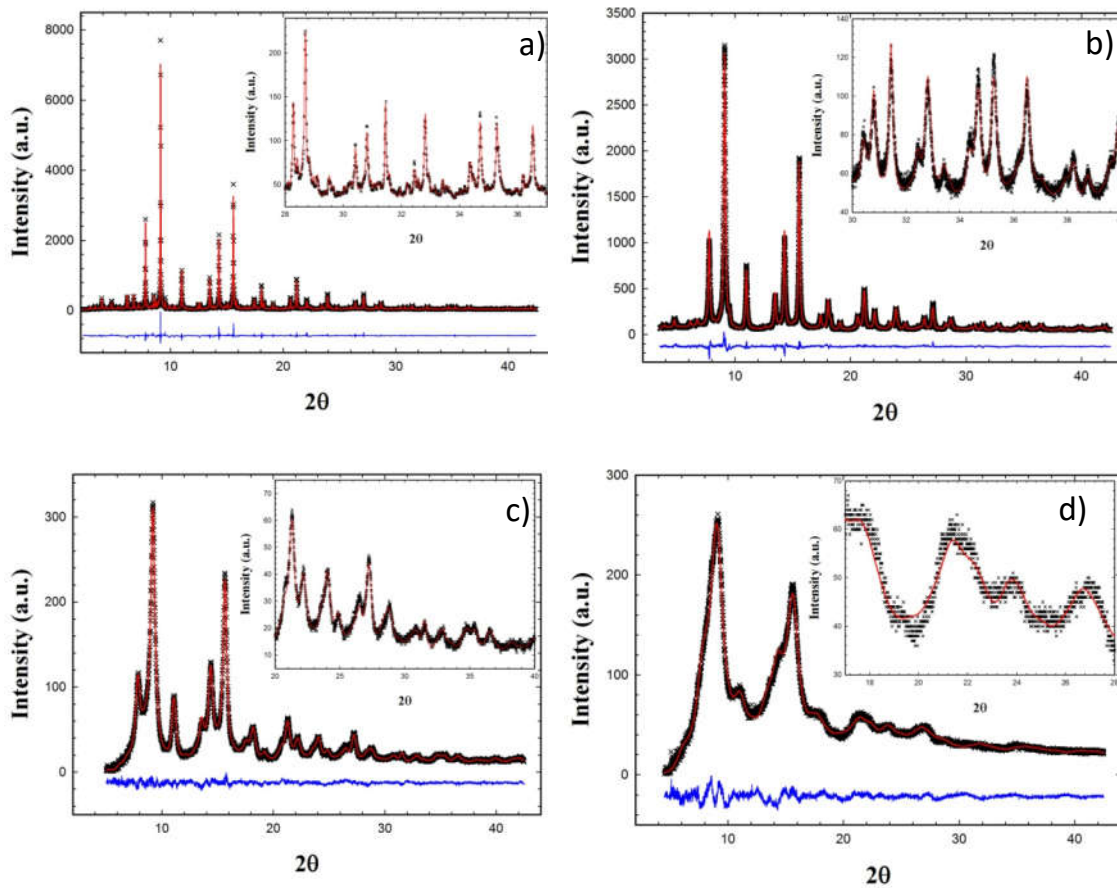


Figure S7. Rietveld refinements for Aldrich (a), Iolitec (b), P520 (c) and P200 (d) samples. Experimental pattern (black crosses), fit (red curves) and differential (blue line) are reported. In the insets the high 2θ range is highlighted.

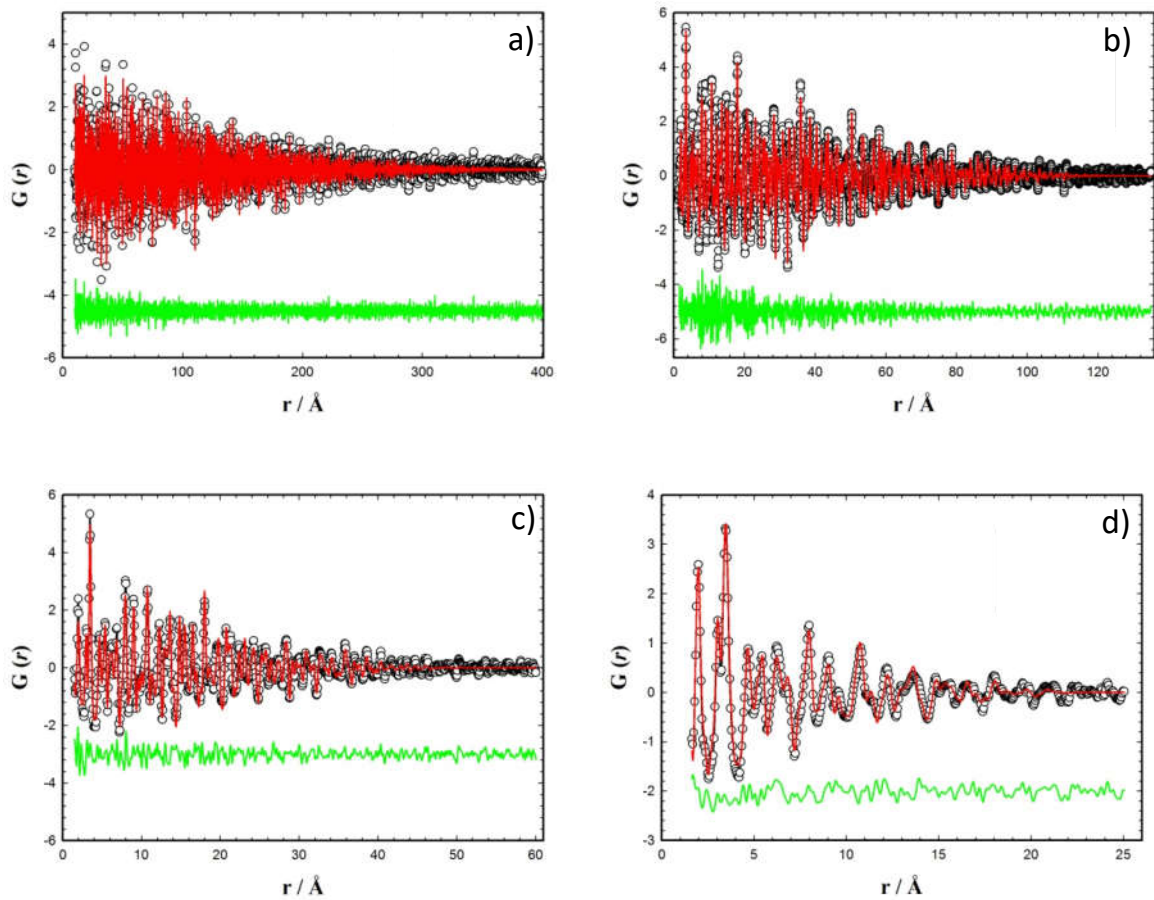


Figure S8. PDF refinements for Aldrich (a), Iolite (b), P520 (d) and P200 (e) samples. Experimental pattern (black symbols), fit (red curves) and differential (green line) are reported.

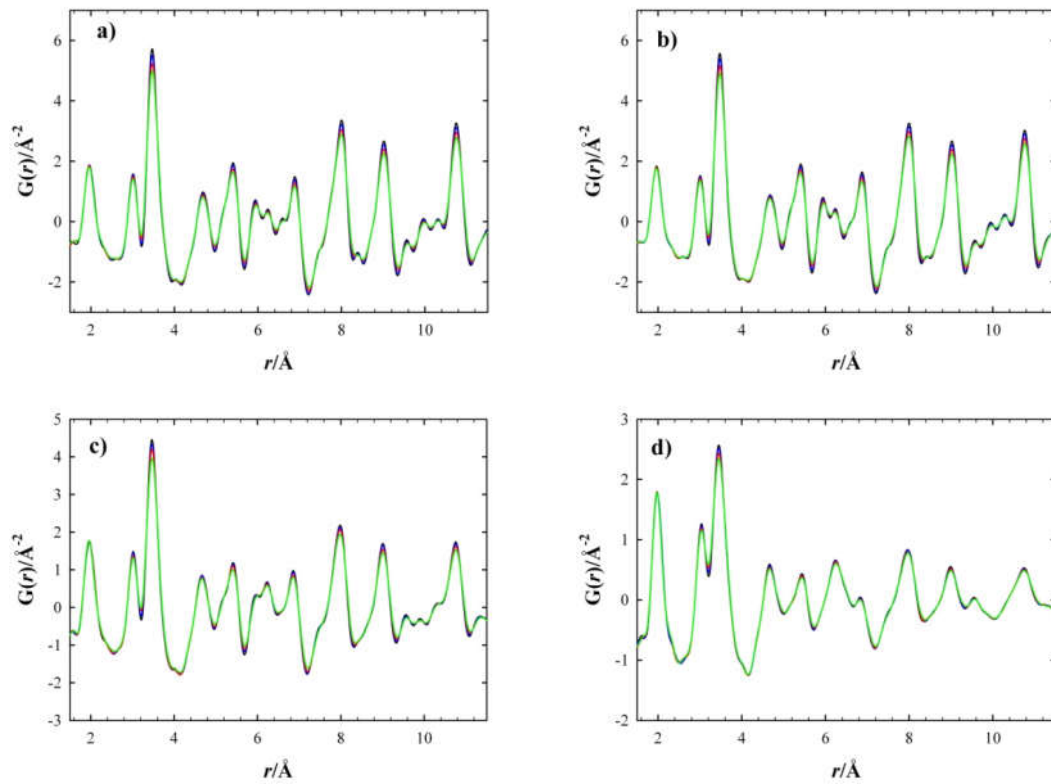


Figure S9. Experimental PDF of Aldrich (a), Iolitec (b), P520 (c) and P200 (d) samples at 120K (black), 180 K (blue), 240 K (red) and 295 K (green).

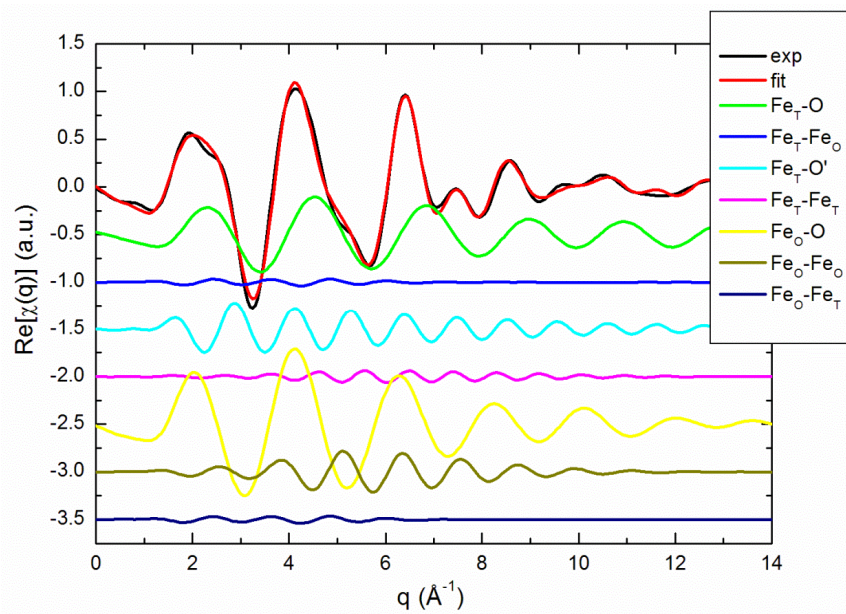


Figure S10a. Back Fourier transform best-fit curve and single contributions for sample P200.

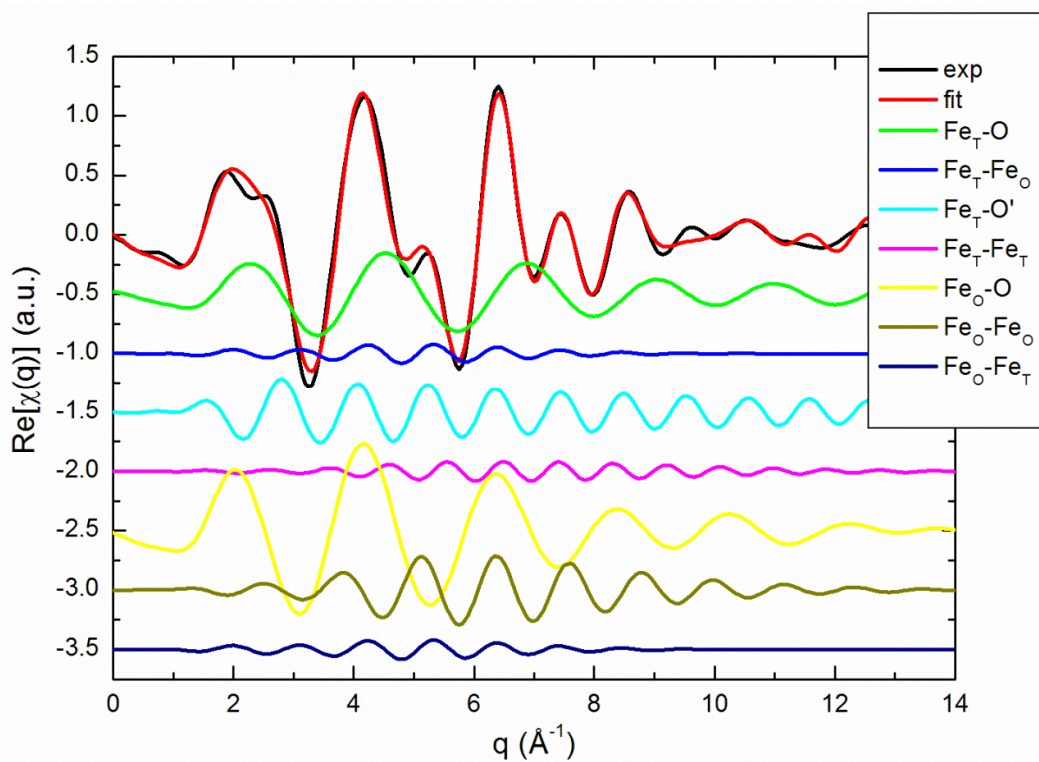


Figure S10b. Back Fourier transform best-fit curve and single contributions for sample P520.

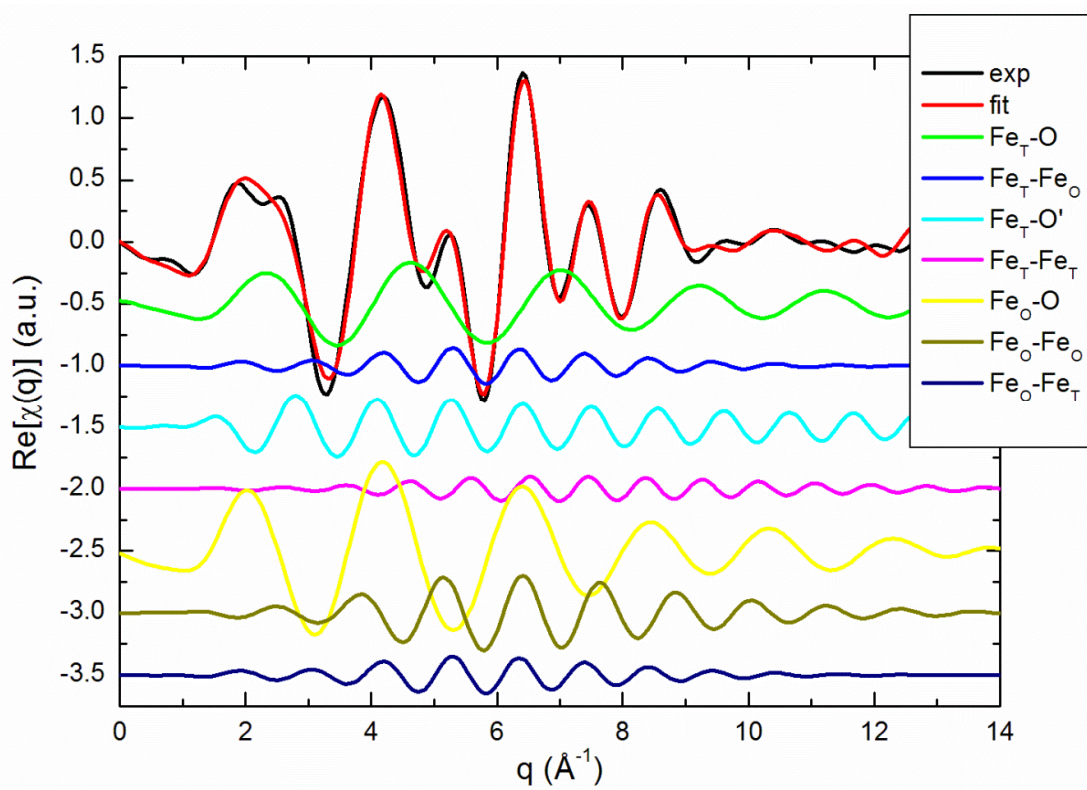


Figure S10c. Back Fourier transform best-fit curve and single contributions for sample Iolitec.

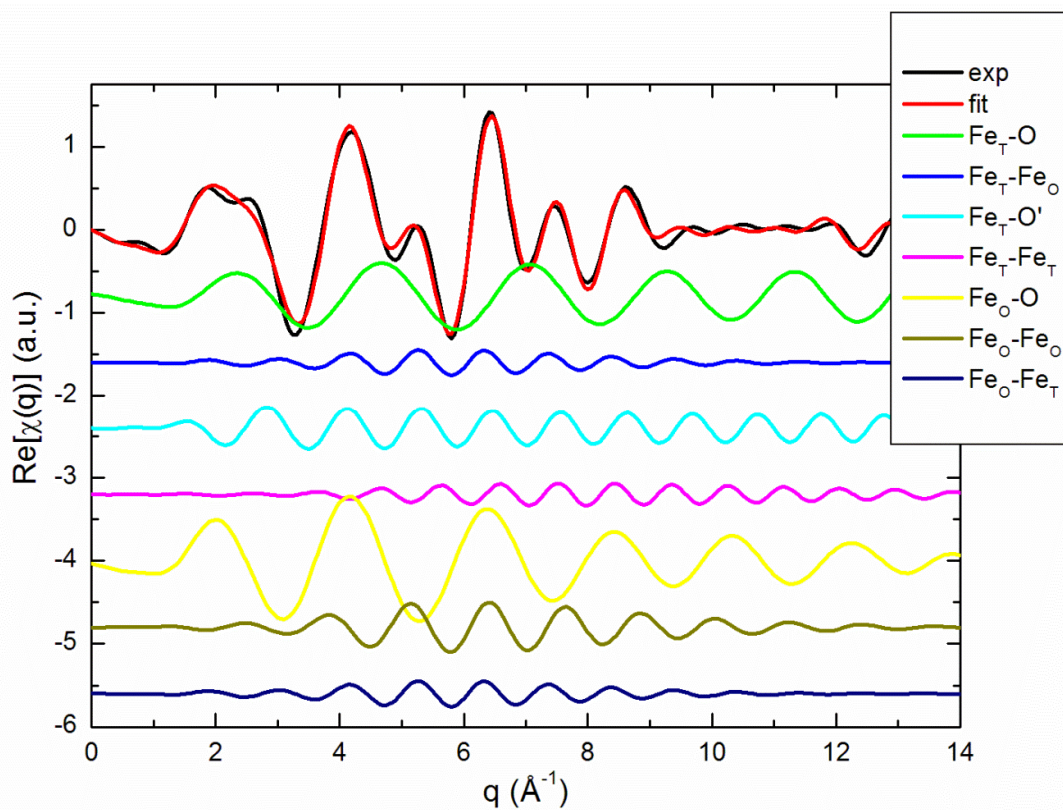


Figure S10d. Back Fourier transform best-fit curve and single contributions for sample Aldrich.

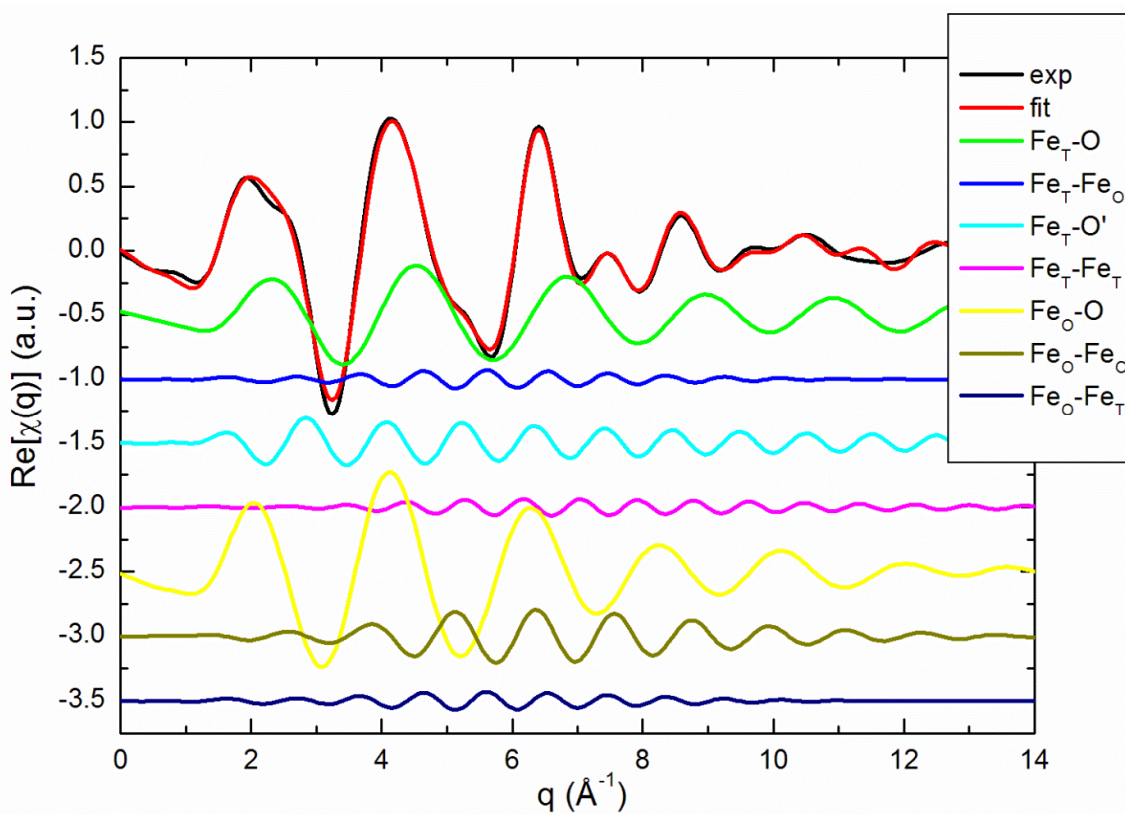


Figure S10e. Back Fourier transform best-fit curve and single contributions for sample P200 with the new coordination number CN' values.

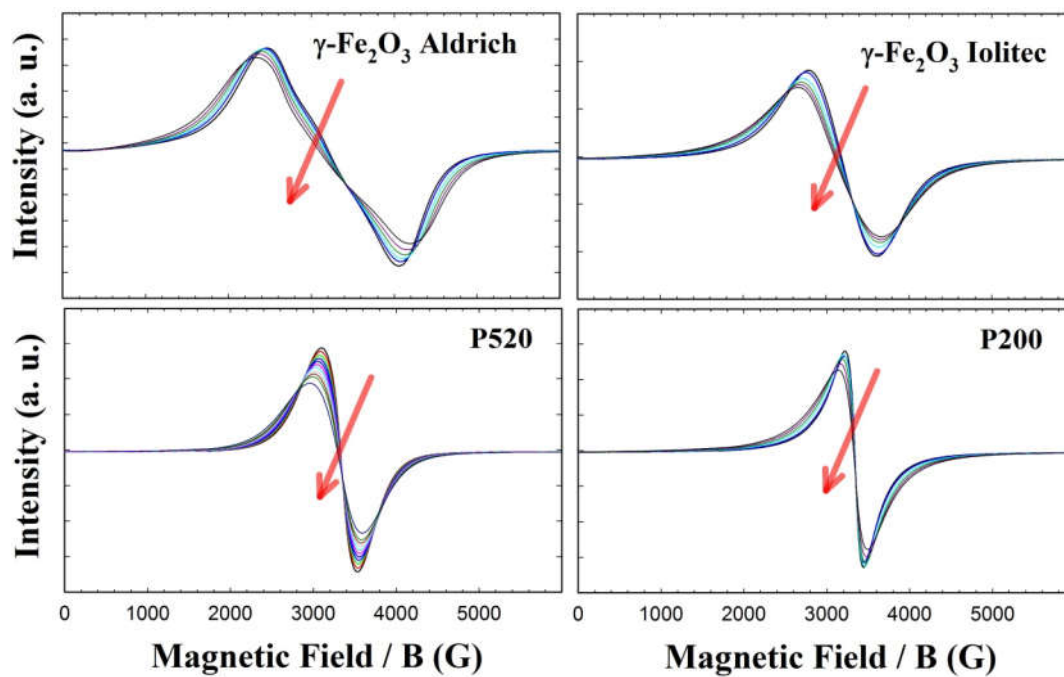


Figure S11. EMR spectra of $\gamma\text{-Fe}_2\text{O}_3$ samples heating up to 420 K. Red arrows indicate heating.