


Supplementary Materials: Experimental and Simulation Studies on the Mn Oxidation State Evolution of a $\text{Li}_2\text{O-MnO}_x\text{-CaO-SiO}_2$ Slag Analogue

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1. Correlation of edge jump and R factor from micro-XANES

The fit errors and edge jumps of LCF from micro-XANES are given with their respective in Figure S1. The median R factor is determined with $R = 0.007$ (25 % percentile at 0.005, 75 % percentile at 0.015). The regions with higher fit errors (R factor > 75 % percentile) correlate with low concentrations (edge-jump < 25 % percentile). The same can be visualized with the 50 % percentiles for R factor and edge-jump (panel D). Direct correlation of low edge jump and high R factor is visible in white color. Areas in blue correspond to high edge jump and low R factor yielding the best LCF results. In pink high R factor areas are denoted while in turquoise low edge jump areas are given.

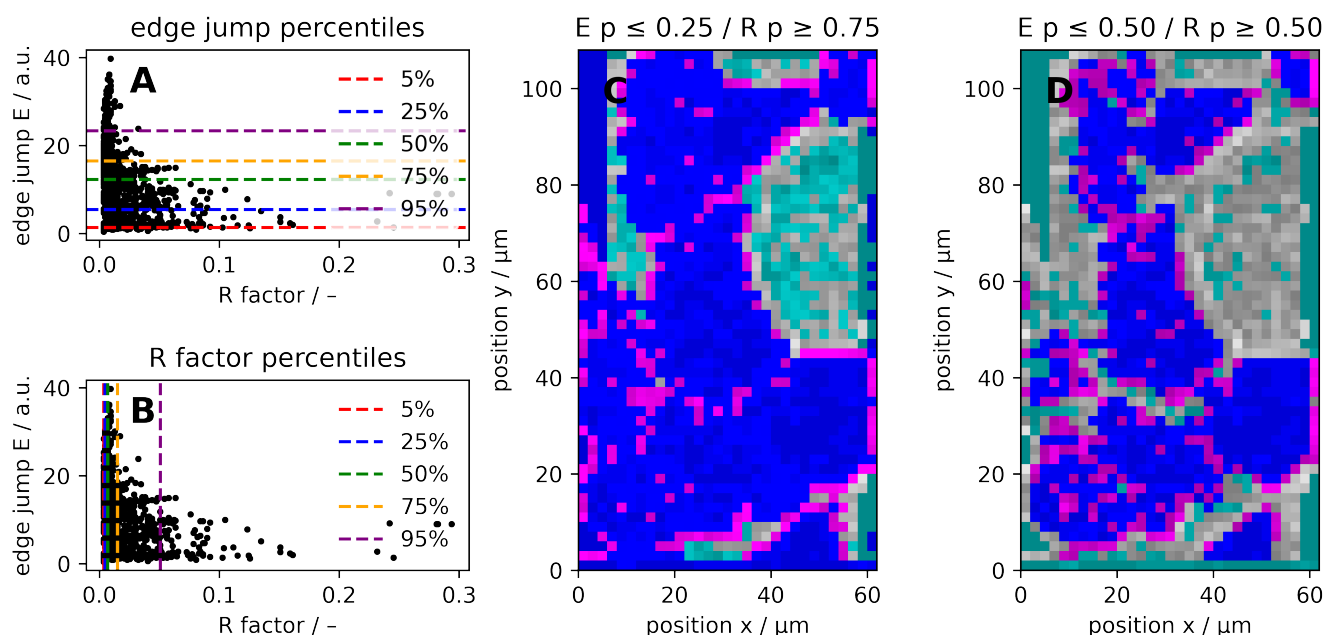


Figure S1. R factors and edge jumps from micro-XANES and micro-XANES linear combination fit (LCF). A: percentiles of edge jump. B: percentiles of R factor. C: false-color image of R factor with data (blue), upper 25% percentile of R factor, and lower 25% percentile of the edge jump. D: false-color image of R factor with data (blue), upper 50% percentile of R factor, and lower 50% percentile of the edge jump.

2. Radial distribution function from MD simulations

The radial distribution function (RDF) is shown in figure S2 for LiMnO_2 and Ca_2SiO_4 at 2100 K and 2400 K, respectively.

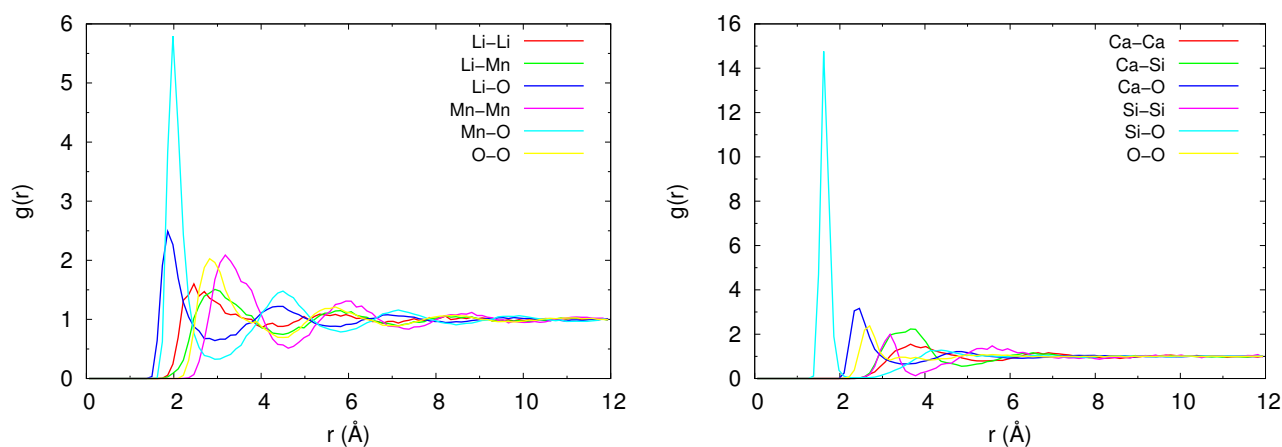


Figure S2. Radial distribution function (RDF) for the different ions in LiMnO_2 at 2100 K (left) and Ca_2SiO_4 at 2400 K (right).

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