

Supplemental material

I. EXAFS FITS

EXAFS fittings were carried out using Larch [1] and a theoretical $\chi(k)$ function was generated by performing ab initio calculations using the FEFF 8 code.[2–4] In the following spectra, the k-space plots and fits are shown at the three edges (Mn, Co, Ni) for all three materials NMC111, NMC622, and NMC811.

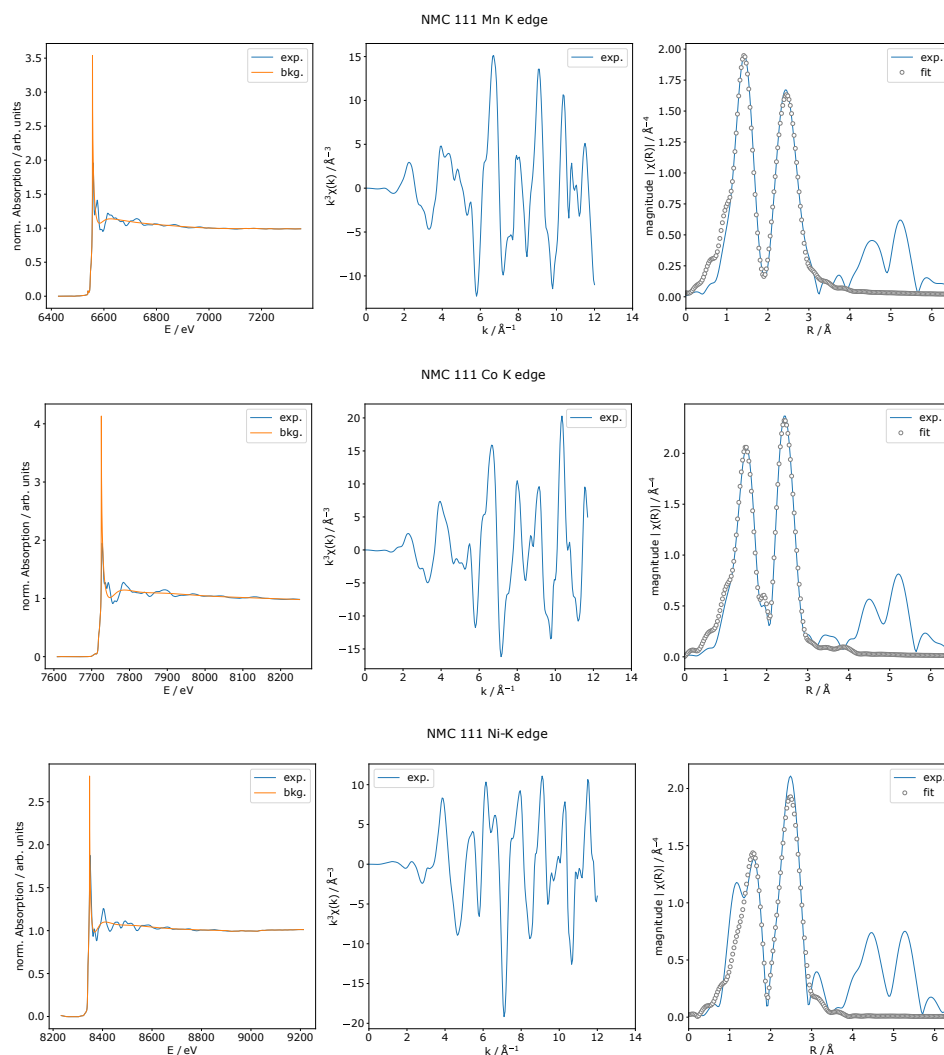


Figure 1. The comparison of NMC111 EXAFS measurement results at the Mn K, Co K, and Ni K edges. The first graph for each edge is the measured EXAFS spectrum with the subtracted background specified. The second graph is the k^3 -weighted $\chi(k)$ EXAFS signal and the third is the magnitude of the Fourier transform.

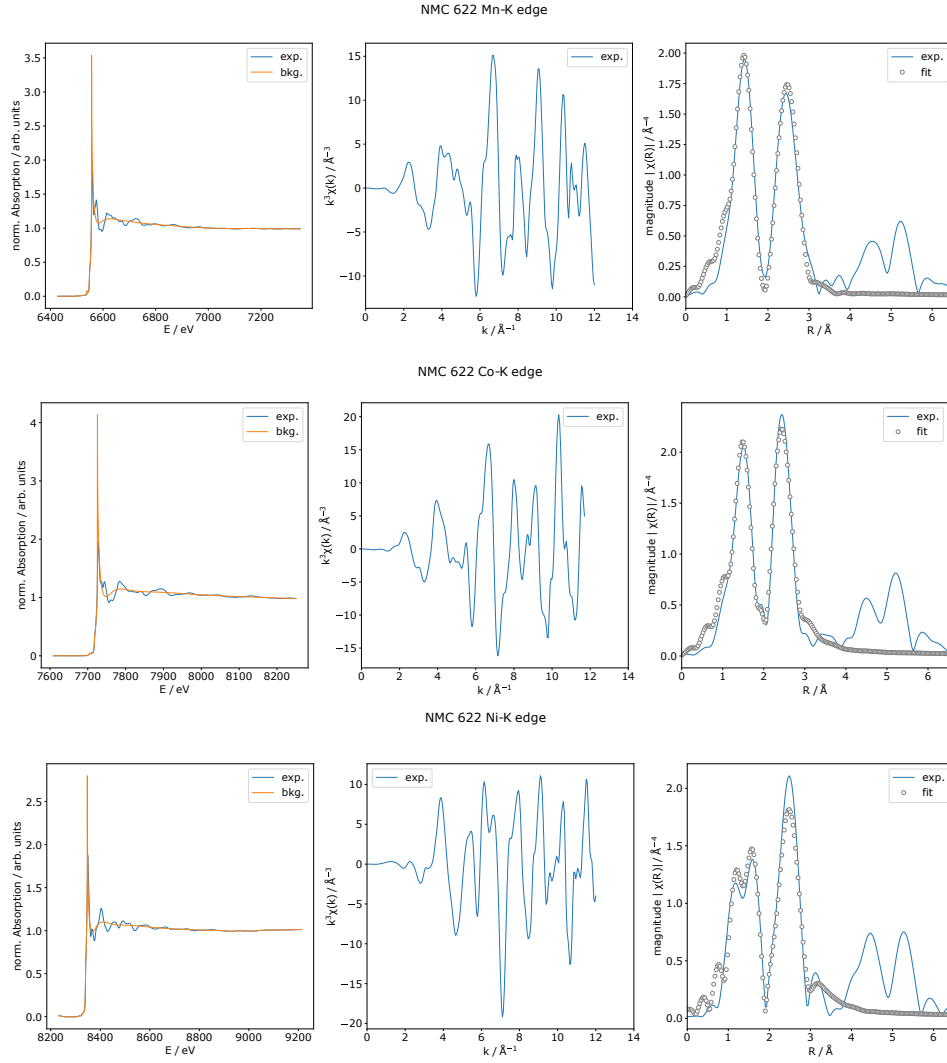


Figure 2. The comparison of NMC622 EXAFS measurement results at the Mn K, Co K, and Ni K edges. The first graph for each edge is the measured EXAFS spectrum with the subtracted background specified. The second graph is the k^3 -weighted $\chi(k)$ EXAFS signal and the third is the magnitude of the Fourier transform.

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- [1] M. Newville, Larch: An Analysis Package for XAFS and Related Spectroscopies, [Journal of Physics: Conference Series](#) **430**, 012007 (2013).
 - [2] A. L. Ankudinov, B. Ravel, J. J. Rehr, and S. D. Conradson, Real-space multiple-scattering calculation and interpretation of x-ray-absorption near-edge structure, [Physical Review B](#) **58**, 7565 (1998).
 - [3] J. J. Rehr and R. C. Albers, Theoretical approaches to x-ray absorption fine structure, [Reviews of Modern Physics](#) **72**, 621 (2000).
 - [4] J. J. Rehr, J. J. Kas, M. P. Prange, A. P. Sorini, Y. Takimoto, and F. Vila, Ab initio theory and calculations of X-ray spectra, [Comptes Rendus Physique](#) **10**, 548 (2009).

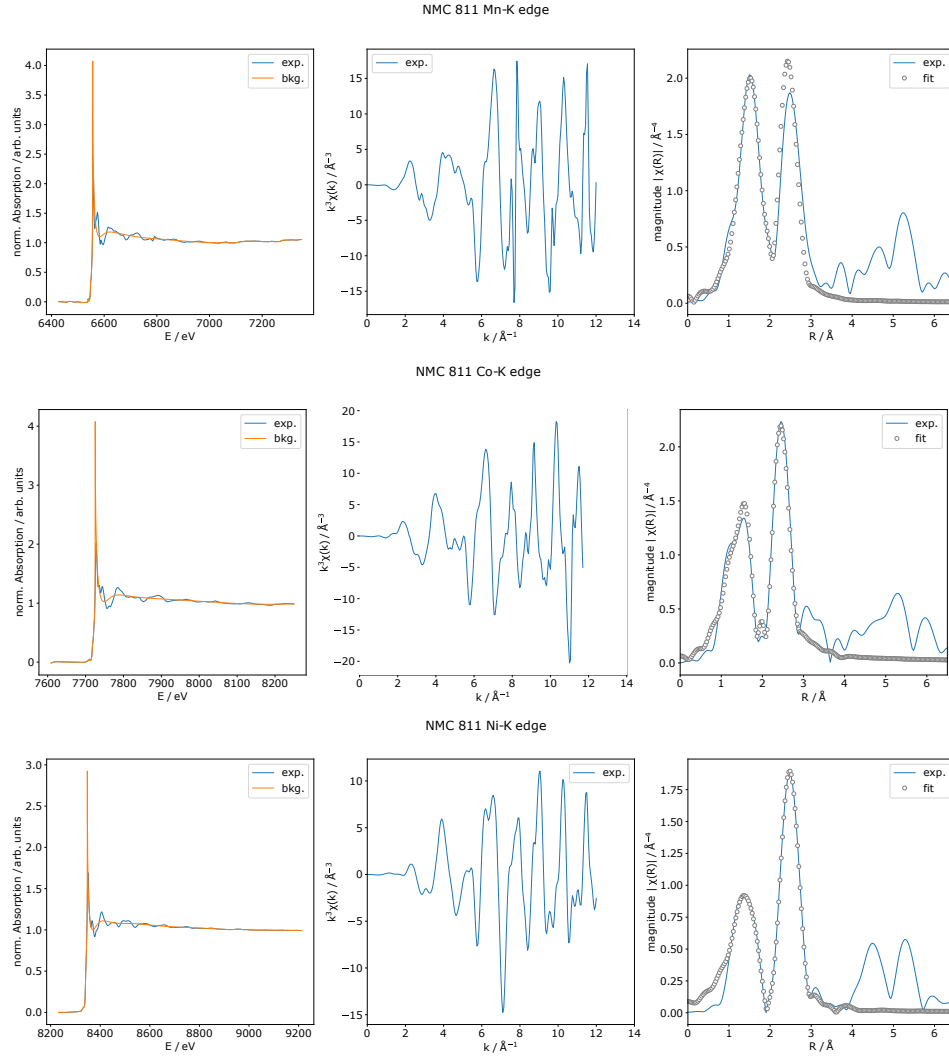


Figure 3. The comparison of NMC811 EXAFS measurement results at the Mn K, Co K, and Ni K edges. The first graph for each edge is the measured EXAFS spectrum with the subtracted background specified. The second graph is the k^3 -weighted $\chi(k)$ EXAFS signal and the third is the magnitude of the Fourier transform.