Erratum: Intrinsic structure of relaxor ferroelectrics from first principles [Phys. Rev. B 114, 024204 (2026)]

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In the implementation employed to compute the neutron total-scattering structure factor $S(Q)$, the neutron scattering length of Mg ($b_{\mathrm{Mg}} = 5.375$ fm) was incorrectly set to the value corresponding to Mn ($b_{\mathrm{Mn}} = -3.750$ fm), which was reflected by Ref. [61] of the original article. This incorrect value of the scattering length was used in the computation of the simulated structure factor $S(Q)$ and the corresponding pair distribution function $H(r)$, as shown in the upper panel of Fig. 3 of the original article, which is reproduced here in Fig. 1(a).

Employing the appropriate Mg scattering length yields a recalculated neutron-scattering intensity in which both the peak positions and their relative magnitudes exhibit slight shifts. The revised, corrected results are presented in Fig. 1(b). The corrected results exhibit improved consistency with the experimental measurements, both with respect to the peak positions and the profiles of the line shapes. The remaining discrepancy should be primarily attributed to errors in the density functional approximation. This finding provides additional validation of the FIRE-Swap methodology and its first-principles-based predictive capability, which operates independently of any refinement using experimental data.

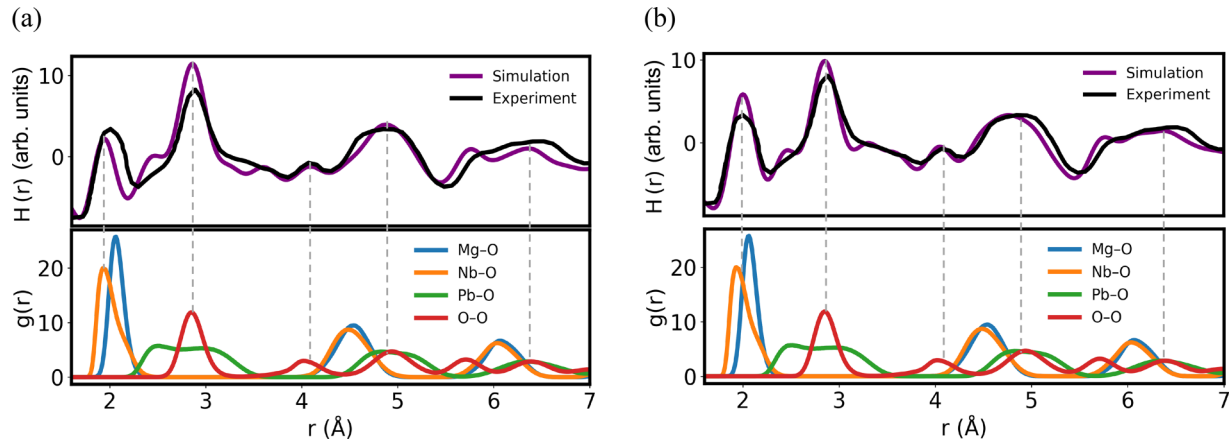

FIG. 1. (a) $H(r)$ calculated using an incorrect Mg bound coherent neutron scattering length, $b_{\mathrm{Mg}} = b_{\mathrm{Mn}} = -3.750$ fm. Reproduced from the original article, and (b) the corrected $H(r)$ calculated using $b_{\mathrm{Mg}} = 5.375$ fm. In the upper panels, purple and black curves denote the calculated and experimental $H(r)$, respectively. The lower panels show the calculated partial radial distribution functions.