Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary information

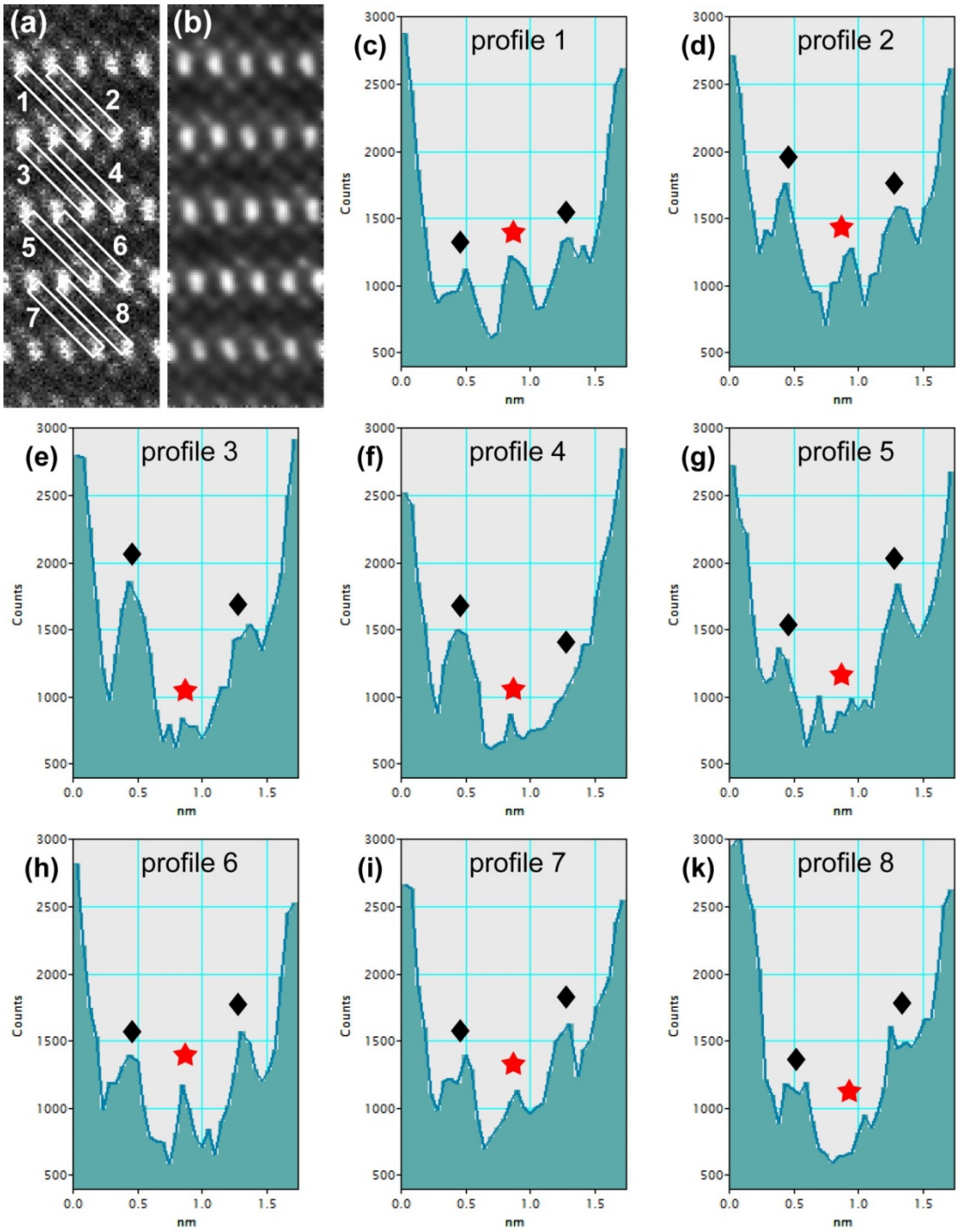

Figure S1. (a) Experimental Fe STEM-EELS elemental map. (b) The same map after low-pass filtering. This operation significantly reduces the noise and hence improving visual interpretation of the image. (c-k) Intensity profiles measured on the experimental Fe-map along the [100] direction of the basic perovskite structure. The exact position, where the profiles were measured is indicated with the rectangles in figure (a). On the profiles, black diamonds indicate the B2

position, and red stars – the B3 positions. According to the profiles, the Fe occupancy in the B2 positions on average is significantly higher than in the B3 positions.

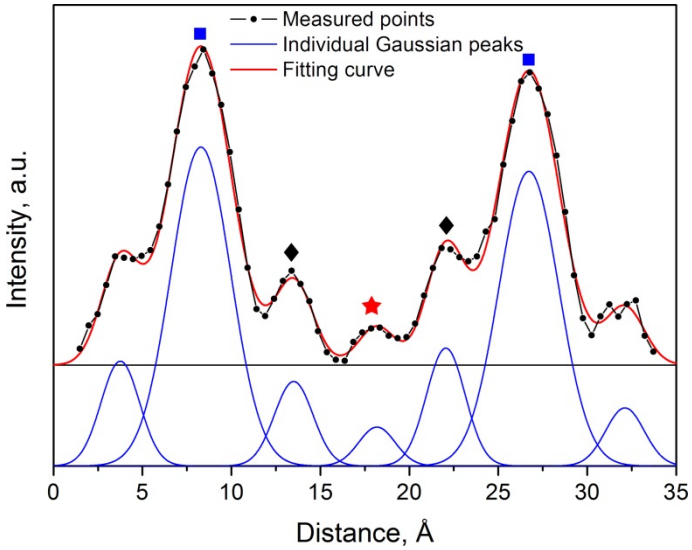

Figure S2. An averaged intensity profile of the Fe STEM-EELS elemental map (Figure S1a). For averaging, 12 individual [100] profiles were measured (similar to those in Figure S1), aligned with respect to the position of the peaks and summed up. B1-positions are indicated with the blue squares, the B2 – with black diamonds, the B3 – with a red star. The measured data were fitted with a set of Gaussian functions above a constant background. Because of the specific interaction of the electron beam with the crystalline matter, the intensity of the peaks can be treated qualitatively only. They confirm that the majority of Fe occupies tetragonal pyramids (the B1-sites) and minor fraction of Fe is present in both octahedral positions with prevalence in B2 rather than B3.

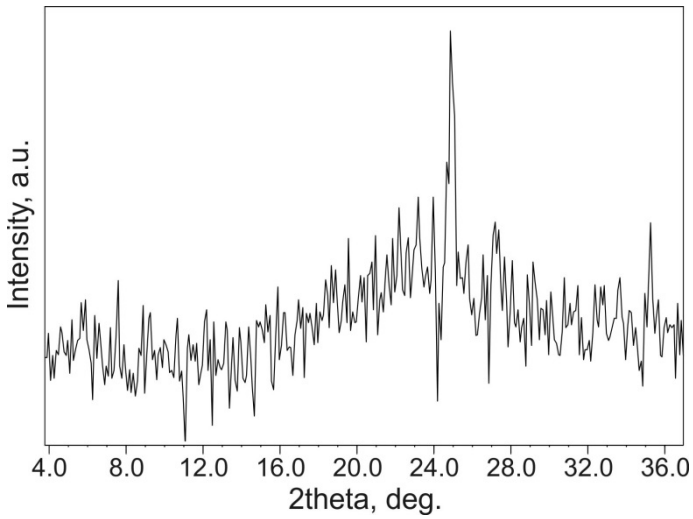

Figure S3. Difference curve between the RT and LT NPD data (λ = 1.8857 Å). One can notice the presence of weak diffuse intensity centered near 2θ = 23º. The sharp spike is a residual after the subtraction of the (006) nuclear reflection (2θ = 24.10º).

TOC image