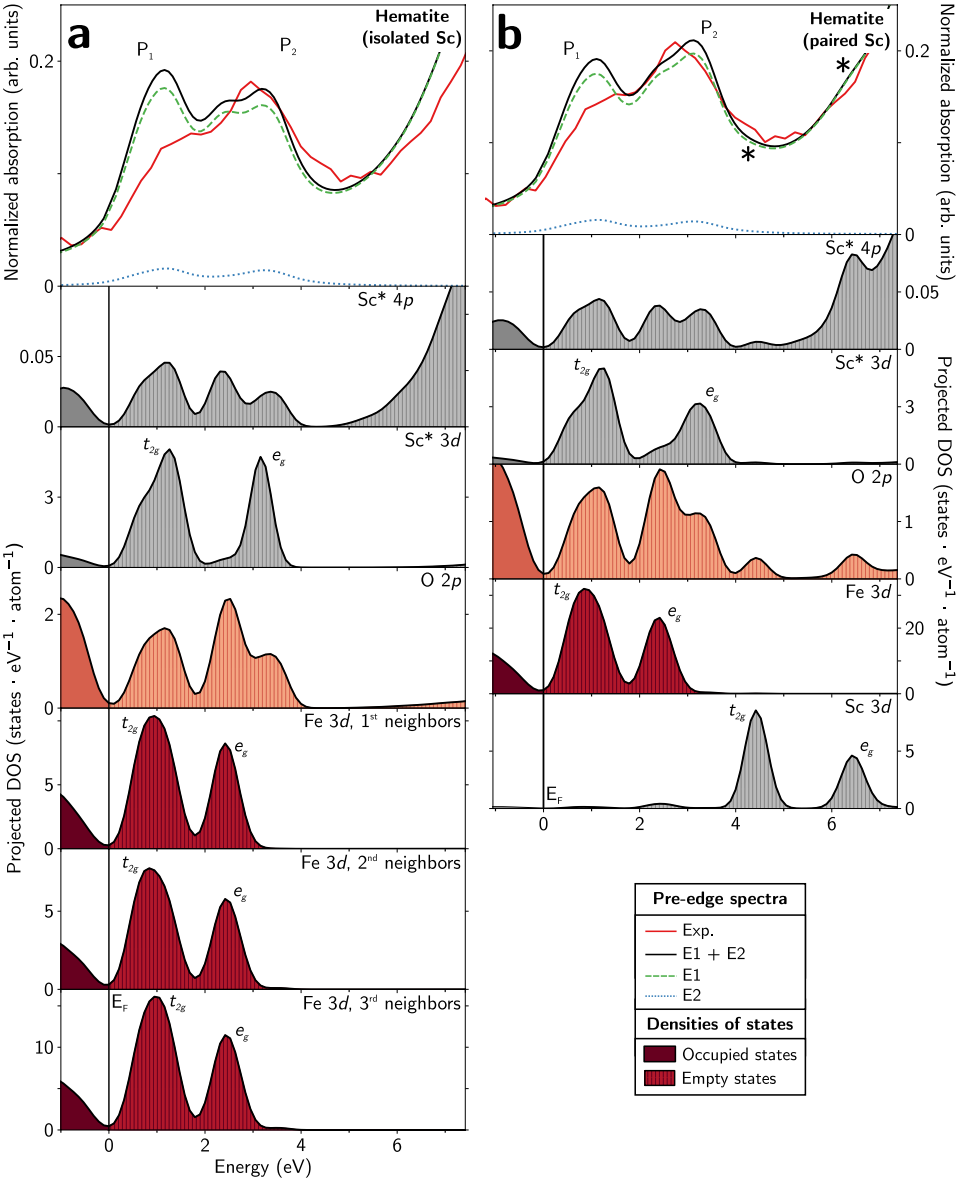
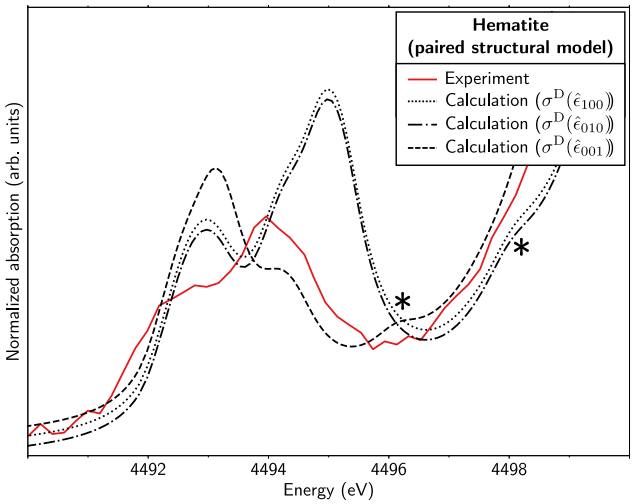


Supplemental Figure S1. Experimental and calculated pre-edge regions of Sc *K*-edge XANES spectra of Sc-substituted hematite: (a) isolated structural model; (b) paired structural model. The calculated electric dipole (E1) and quadrupole (E2) contributions are displayed. The partial densities of the absorbing Sc (Sc*) 4*p* and 3*d* states, of the first six O neighbors 2*p* states, of the first Fe and Sc neighbors 3*d* states are shown. In a matter of clarity, the DOS from the three clusters of Fe neighbors in hematite located at ca. 3.0 Å, ca. 3.4 Å and ca. 3.7 Å are averaged, due to their similarities. The energy scale of the experimental spectra is shifted to match calculated spectra. The vertical line indicates the Fermi level (E_F). The * symbols indicate features discussed in the paper.



SUPPLEMENTAL FIGURE S2. Comparison between experimental (red) and calculated (black) normalized Sc pre-*K*-edge XANES spectra of Sc-substituted hematite (paired structural model). Each calculated spectrum corresponds to the electric-dipole cross section for a given orientation of the polarization vector ($\hat{\epsilon}$) chosen in an orthonormal reference frame bound to the crystal.