Supplementary Electronic Information on Pb Speciation using EXAFS and XANES.

Figures S-1 to S-3 illustrate the evolution of the XANES and EXAFS spectra reflecting changes in Pb speciation in two dust samples after 4 months of aging in a humid environment (summarized in Table 3). Figures S-1 to S-2 include FT spectra for comparison with the predicted chi. As indicated in the text, the modeling of the original sample HM112 indicates the presence of some organic Pb species (e.g., Pb citrate or Pb humate) but the exact species could not be resolved. Likewise, the model for the weathered HM112 dust is likely missing a key species, which is indicated by the lack of fit in the hump at around 5 $Å^{-1}$ in the chi data, along with a low sum of fractions before normalization (provided in Table 3). Similar limits were encountered in the fitting of the original NIST 2584 dust sample, where the model predicts only two species but has an overall low sum of fractions before normalization (87.7%; Table 3), which is often an indication that key species are missing. For the weathered NIST 2584 sample, the Pb chromate has a relatively high energy shift (-1.47 eV), which may indicate the existence of species in this fit which are not fully identified. As discussed in the text, the occurrence of Pb naphthenate is interpreted in a general way as an indication of the presence of an organic Pb species with a structure similar to that of Pb naphthenate. For example, Figure S-4 shows similar XANES spectra for Pb adsorbed on humate and Pb naphthenate, as well as comparable features in their EXAFS spectra (relatively same frequencies). Despite these limitations, consistencies in the fits are useful for highlighting major trends in the change of Pb speciation in the dust samples during aging, which provides insight into the observed increase in Pb bioaccessibility.

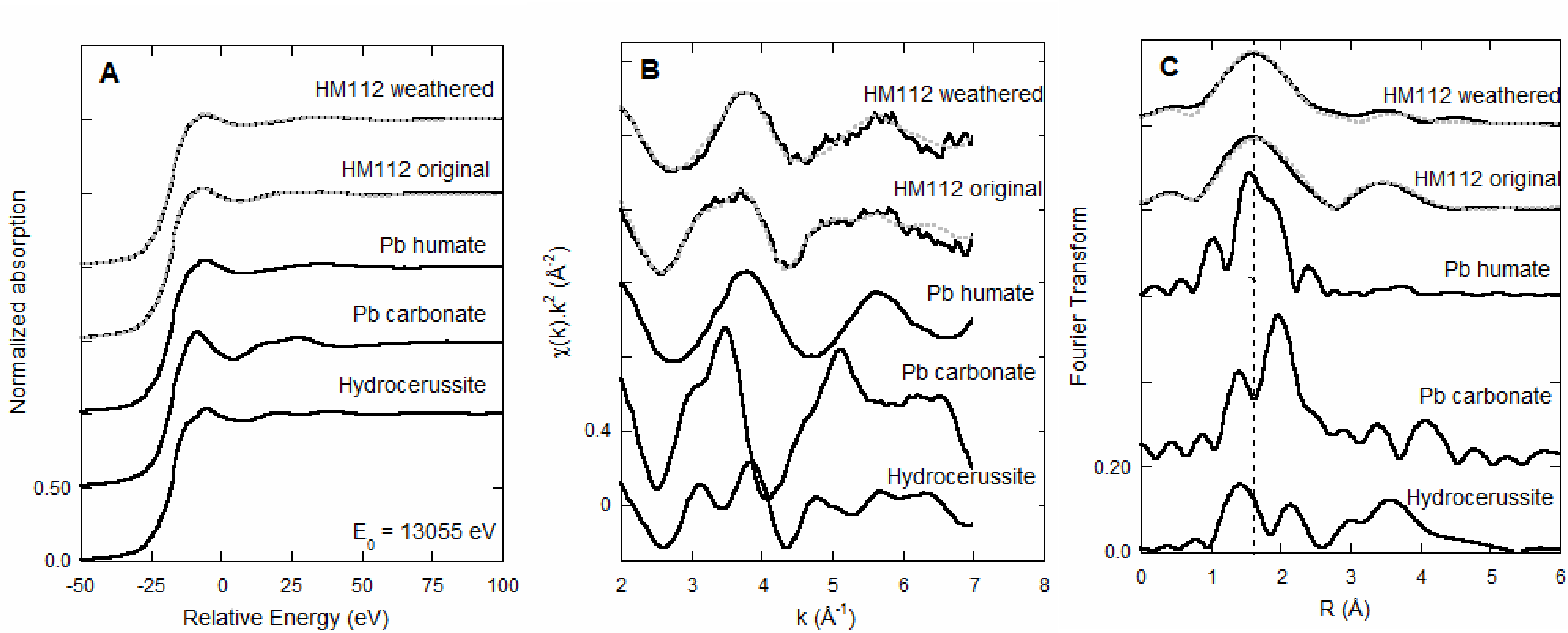
List of Figures

Figure S1. (A) Pb L-111 edge XANES, (B) k^2-weighted EXAFS and (C) Fourier transformed k^2-weighted EXAFS (uncorrected for phase shift) for the original and 4-month weathered HM112 dust (solid black line = measured; dotted grey line = fitted data #1 from Table 3). Reference compounds of hydrocerussite (Pb hydroxyl carbonate), Pb carbonate and Pb adsorbed on humate are illustrated for comparison.

Figure S2. (A) Pb L-111 edge XANES, (B) k^2-weighted EXAFS and (C) Fourier transformed k^2-weighted EXAFS (uncorrected for phase shift) for the original and 4-month weathered N2584 dust (solid black line = measured; dotted grey line = fitted data - Table 3). Reference compounds of hydrocerussite (Pb hydroxyl carbonate), Pb naphthenate and Pb chromate are illustrated for comparison.

Figure S3. Comparison of Pb XANES (A) and EXAFS (B) spectra for house dust HM112 and N2584 before (dark solid line) and after 4-month aging (grey solid line) in an oxygenated, humidity chamber.

Figure S4. Comparison of Pb XANES (A) and EXAFS (B) spectra for Pb naphthenate (dark solid line) and Pb adsorbed on humate (grey solid line).



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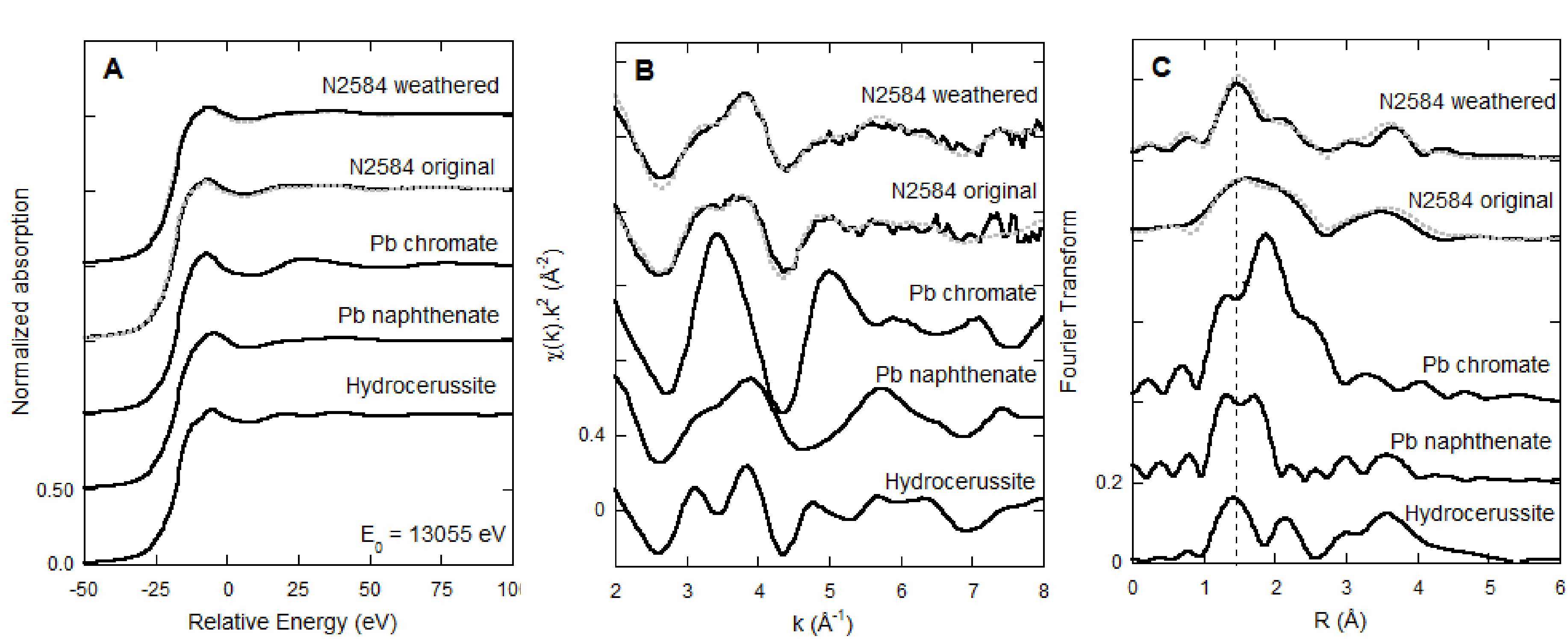

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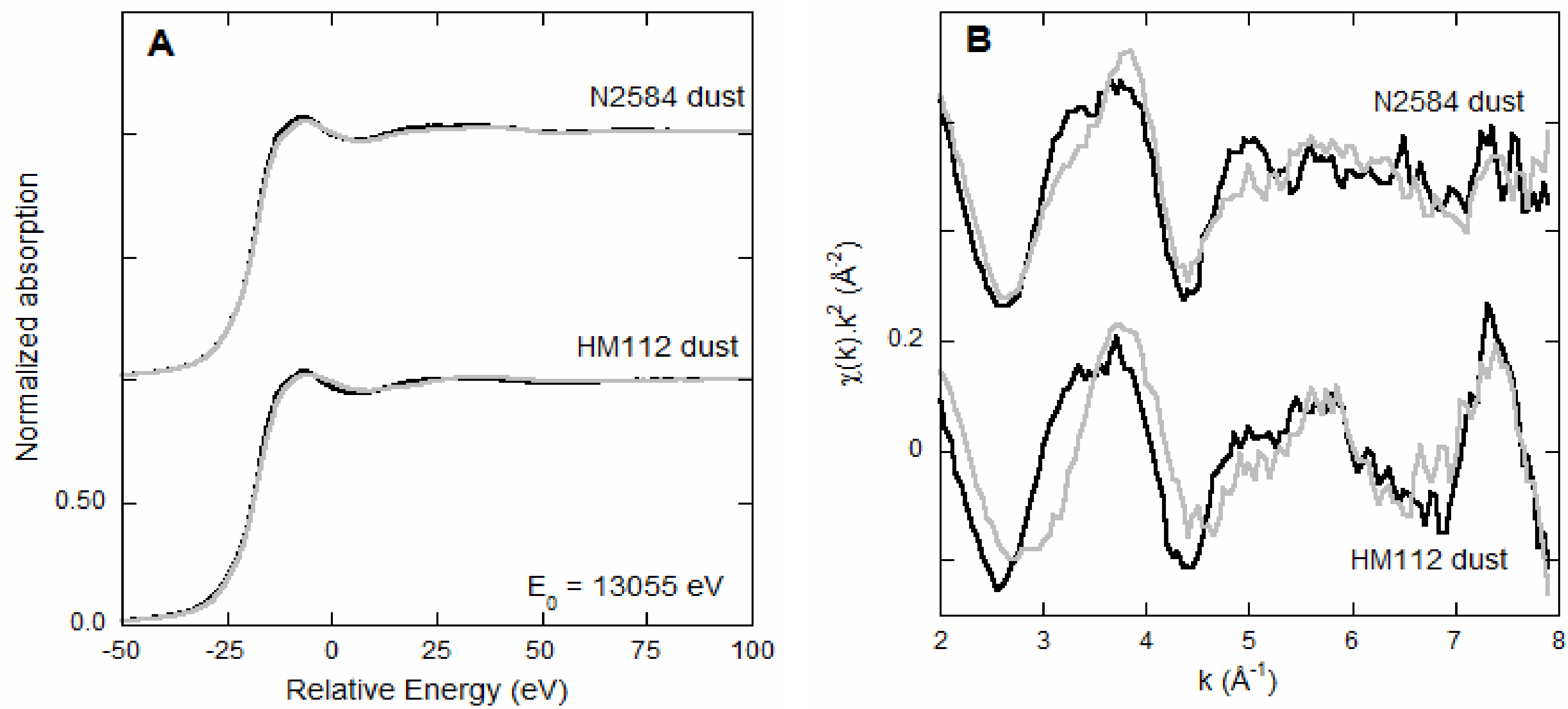

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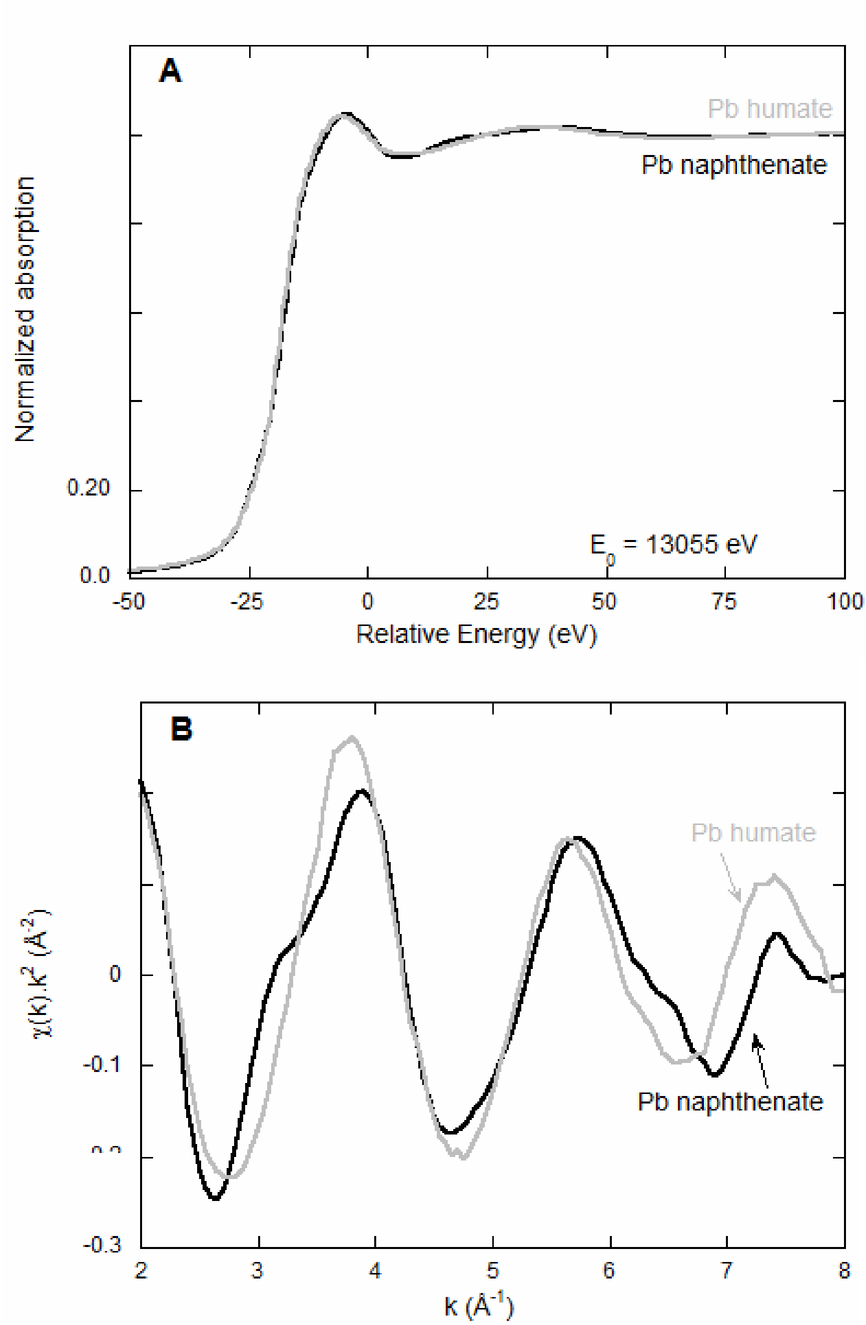

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