Electronic Supplementary Material (ESI) for RSC Advances.

Cubic and Tetragonal Ferrite Crystal Structures for Copper Ion Immobilization in Iron-rich Ceramic Matrix

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Supporting Information

Including 1 table and 8 figures in 10 pages

Table S1. Factors used as goodness-of-fit criteria in the Rietveld refinement.

Criteria of fit	Definition
"R-pattern", R_p	$R_P = \frac{\sum \lvert Y_{o,m} - Y_{c,m} \rvert}{\sum Y_{o,m}}$
"R-weighted pattern", R_{wp}	$R_{WP} = \sqrt{\frac{\sum w_m (Y_{o,m} - Y_{c,m})^2}{w_m {Y_{o,m}}^2}}$
"R-expected", R_{exp}	$R_{exp} = \sqrt{\frac{\sum M - P}{\sum w_m {Y_{o,m}}^2}}$
"Goodness of fit", *GOF*	$GOF = chi^2 = \frac{R_{WP}}{R_{exp}} = \sqrt{\frac{\sum w_m (Y_{o,m} - Y_{c,m})^2}{M - P}}$

where $Y_{o,m}$ and $Y_{c,m}$ are the observed and calculated data, respectively, at data point m; M is the number of data points; P is the number of parameters; and w_m is the weighting given to data point m. The counting statistics is given by $w_m = 1/\delta(Y_{o,m})^2$, where $\delta(Y_{o,m})$ is the error in $Y_{o,m}$. The R_{WP}/R_{exp} ratio or the "goodness of fit (GOF)" value will be equal to one in an ideal refinement. However, in an actual situation, the background and peak profile mismatch lead to GOF>1. A GOF value between 1.0 and 2.9 is generally considered satisfactory*.

* Fansuri, H.; Zhang, D. K.; French, D.; Elcombe, M.; Studer, A. An X-ray and neutron diffraction study of the structure of α-$Bi_2Mo_3O_{12}$ as a catalyst for partial oxidation of propylene to acrolein. *In Proceedings of the CHEMECA symposium.* **2004**, *234*.

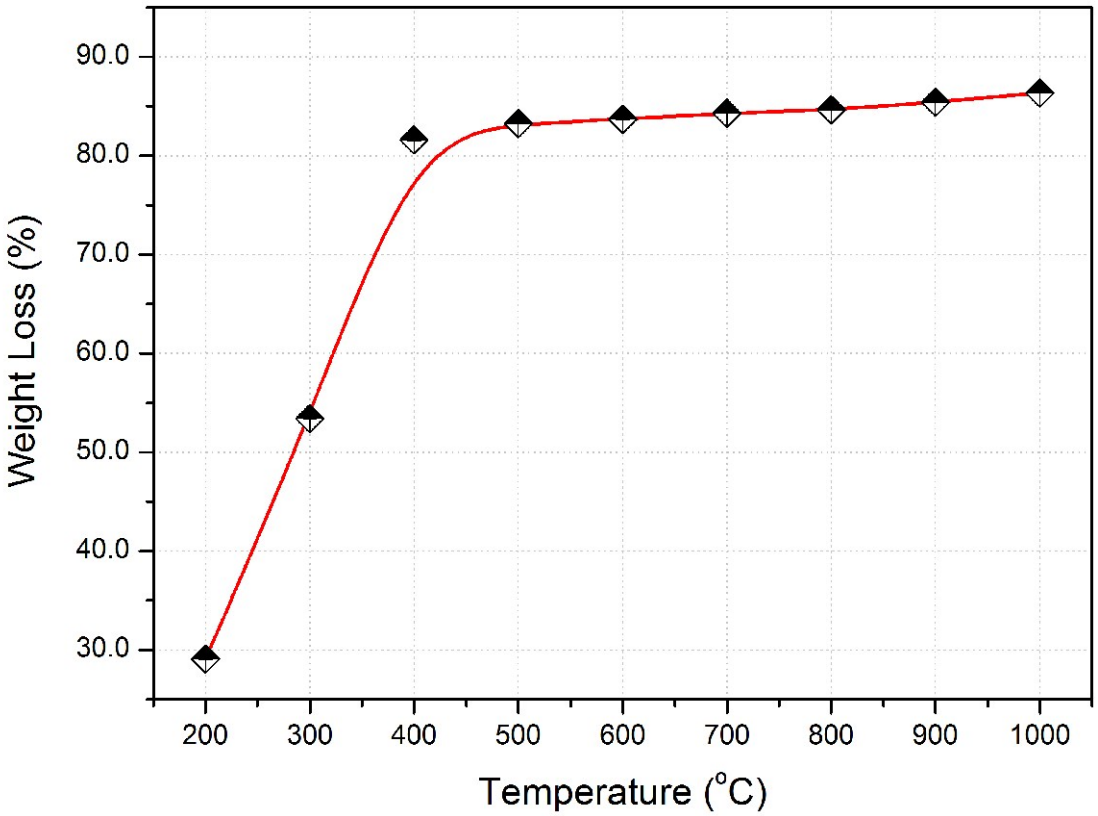

Figure S1. Weight losses of the dried Hong Kong sewage sludge. The dried sludge was prepared by heating the sludge samples overnight at 105 °C. Weight loss measurements were then carried out by heating the dried sludge at designated temperatures for 30 min.

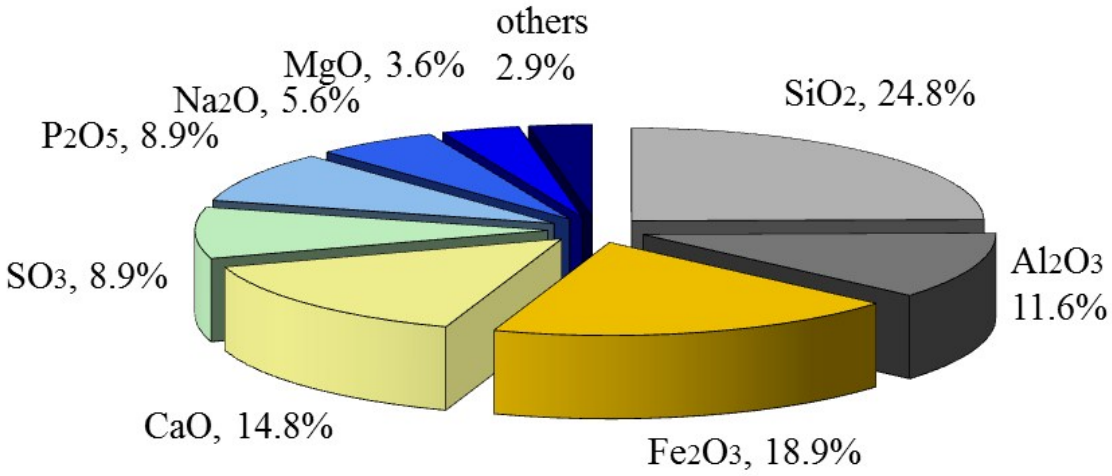

Figure S2**.** Major compositions of the calcined sewage sludge used in the study. The elemental compositions of the 900 ^{o}C and 30-min calcined sewage sludge were analyzed by X-ray fluorescence spectrometry and expressed as the basic oxide forms.

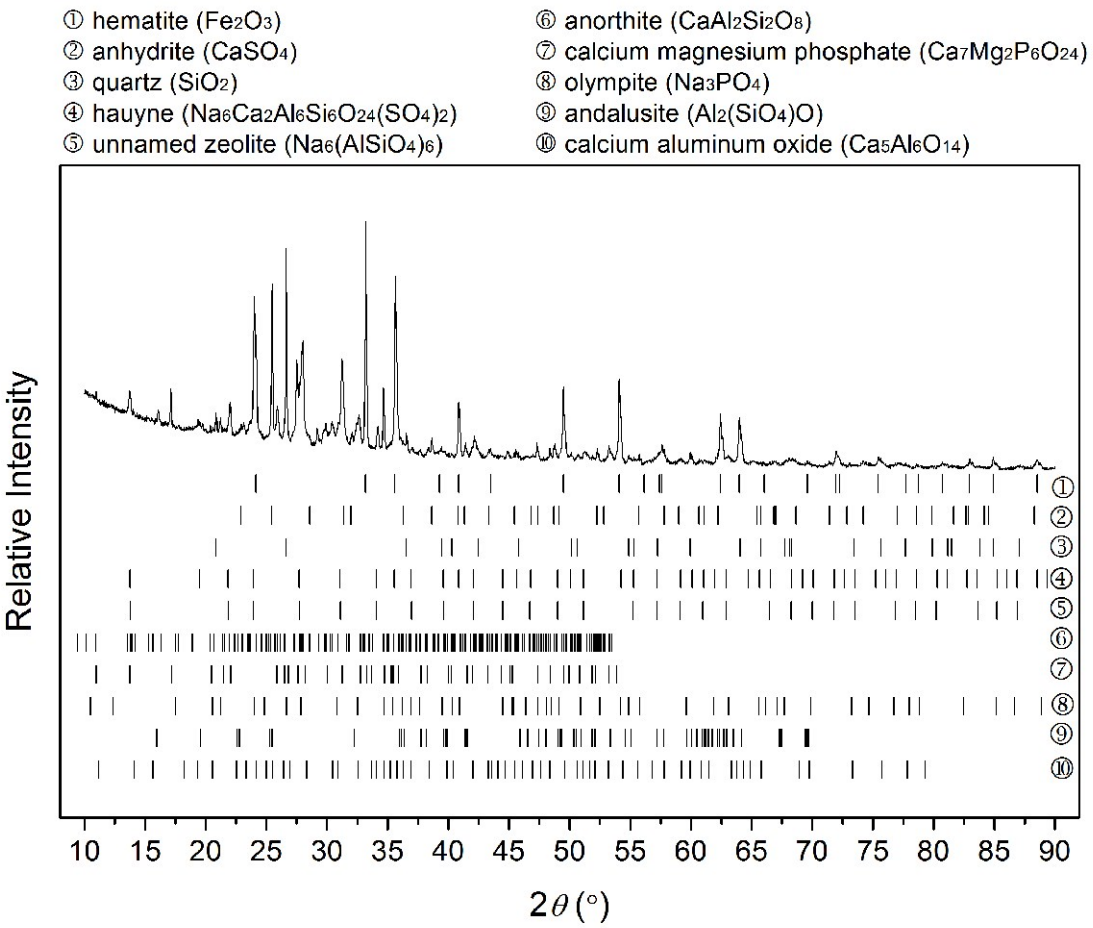

Figure S3. XRD pattern of sewage sludge calcined at 900 °C for 30 min. The crystalline phases are identified as: ☙ hematite (α-Fe_2O_3, PDF#85-0599); & anhydrite ($CaSO_4$, PDF#37-1496); ● quartz (SiO_2, PDF#79-1910); ❍ hauyne ($Na_6Ca_2Al_6Si_6O_{24}(SO_4)_2$, PDF#73-1920); ■ unnamed zeolite ($Na_6(AlSiO_4)_6$, PDF#42-0217); □ anorthite ($Ca(Al_2Si_2O_8)$, PDF#89-1473); ◘ calcium magnesium phosphate ($Ca_7Mg_2P_6O_{24}$, PDF#20-0348); ❑ olympite (Na_3PO_4, PDF#33-1272); ❒ andalusite ($Al_2(SiO_4)O$, PDF#39-0376); ♦ calcium aluminum oxide ($Ca_5Al_6O_{14}$, PDF#11-0357).

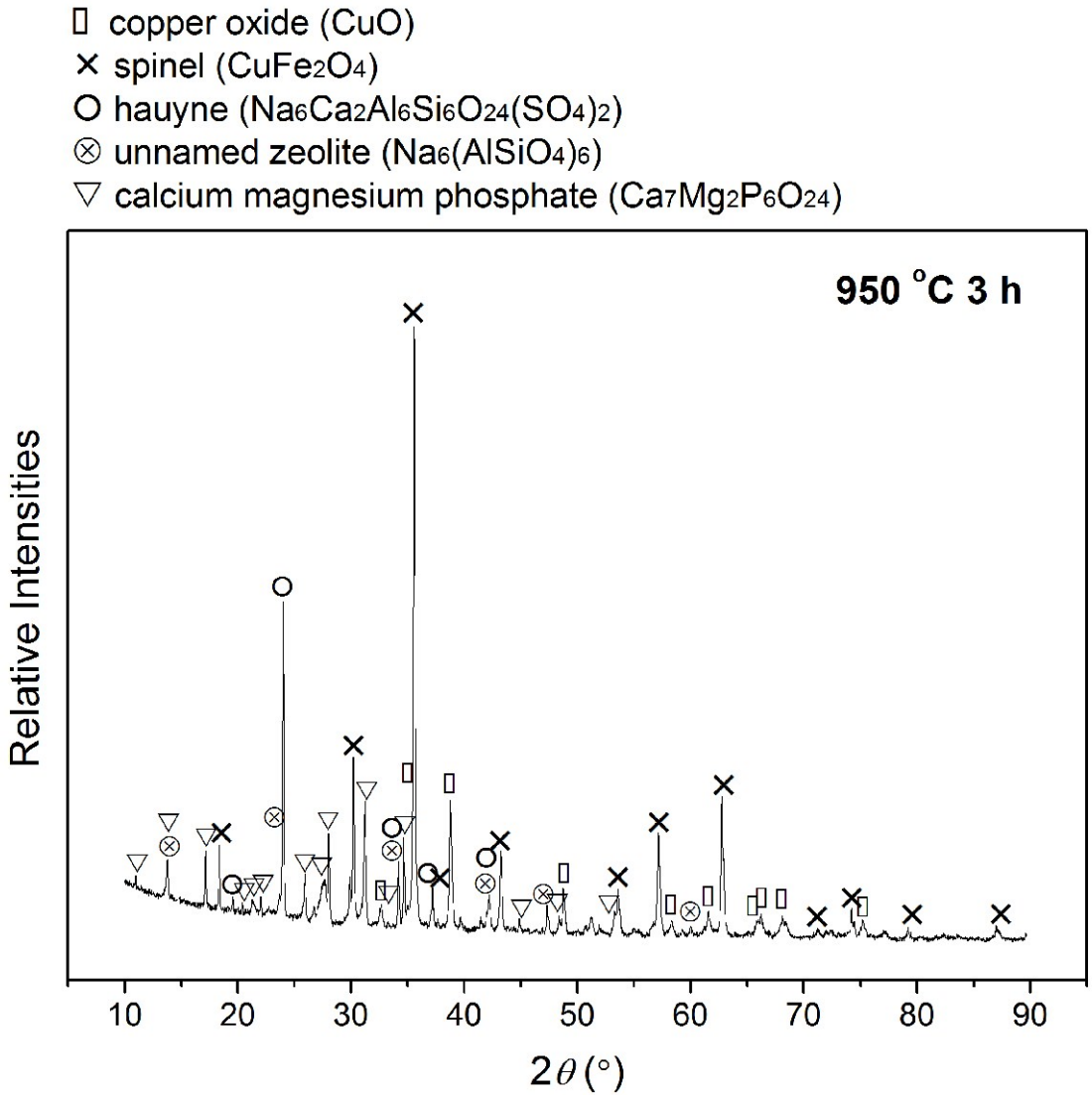

Figure S4. XRD patterns of the CuO + sludge ash (Cu:(Al+Fe) = 1:2) system show the reaction at 950 °C for 3 h. The crystalline phases are identified as: CuO (PDF#80-1268), α-Fe_2O_3 (PDF#85-0599), $CuFe_2O_4$ (PDF#77-0010), anhydrite ($CaSO_4$, PDF#37-1496), quartz (PDF#79-1910), hauyne ($Na_6Ca_2Al_6Si_6O_{24}(SO_4)_2$, PDF#73-1920), unnamed zeolite ($Na_6(AlSiO_4)_6$, PDF#42-0217), anorthite ($Ca(Al_2Si_2O_8)$, PDF#89-1473), calcium magnesium phosphate ($Ca_7Mg_2P_6O_{24}$, PDF#20-0348), calcium aluminum oxide ($Ca_5Al_6O_{14}$, PDF#11-0357), andalusite ($Al_2(SiO_4)O$, PDF#39-0376).

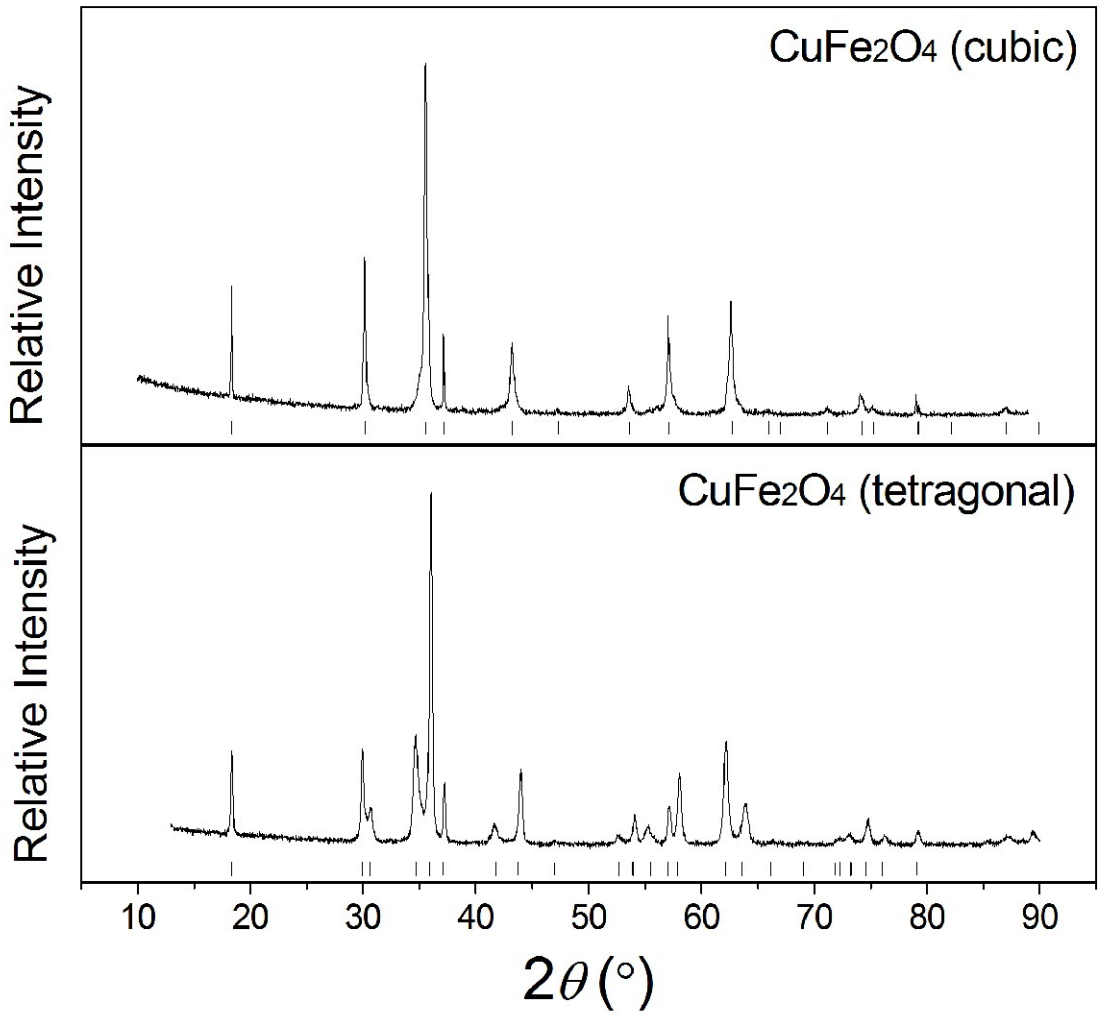

Figure S5. XRD patterns of the single-phase c-$CuFe_2O_4$ (cubic) and t-$CuFe_2O_4$ (tetragonal) samples synthesized for the leaching experiments. The vertical bars at the bottom of the pattern are the standard Bragg positions of c-$CuFe_2O_4$ (PDF#77-0010) and t-$CuFe_2O_4$ (PDF#34-0425).

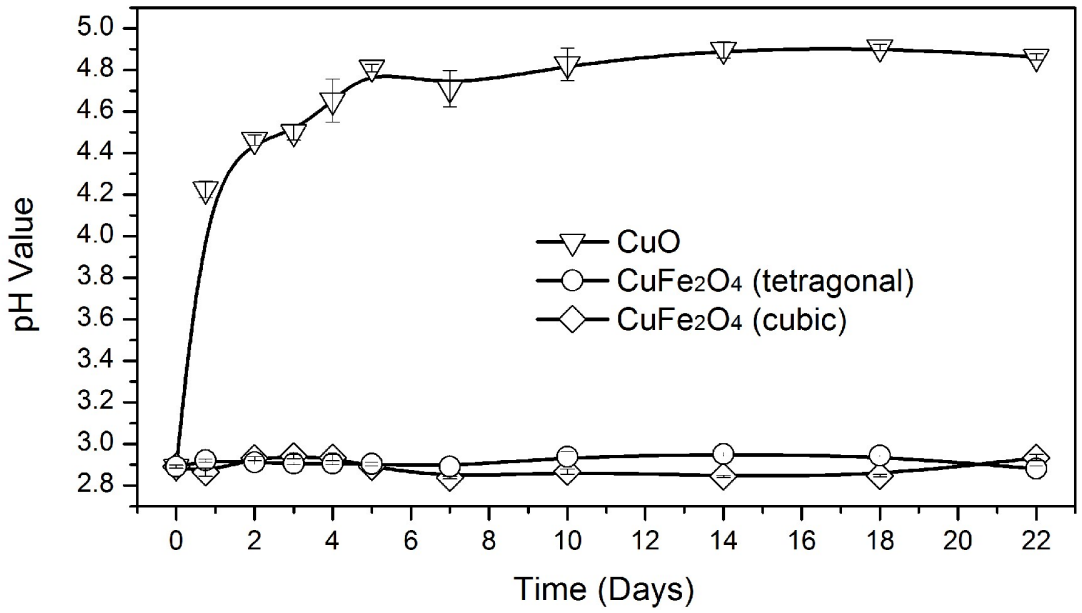

Figure S6. pH values of the CuO, tetragonal $CuFe_2O_4$, and cubic $CuFe_2O_4$ leachates. The leaching solution was TCLP extraction fluid no. 2 (acetic acid solution) with a pH of 2.9. Each leaching vial was filled with 10 ml of extraction fluid and 0.5 g of powder samples, and then rotated end-over-end between 0.75 and 22 d.

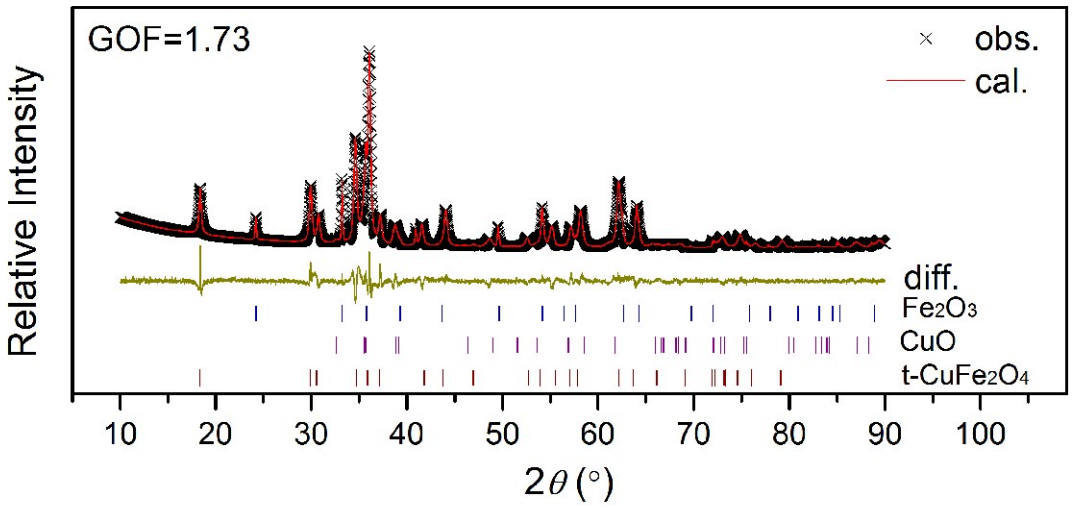

Figure S7. Rietveld refinement result for the product sintered at 750 °C for 3 h from Fe_2O_3 precursor and CuO. The scanned value (obs.), the refined value (cal.) and the difference (diff) are indicated. The standard XRD patterns retrieved from the ICDD database include t-$CuFe_2O_4$ (PDF#34-0425), CuO (PDF#80-1268), and hematite (α-Fe_2O_3, PDF#85-0599). The goodness-of-fit of this refinement is 1.73.

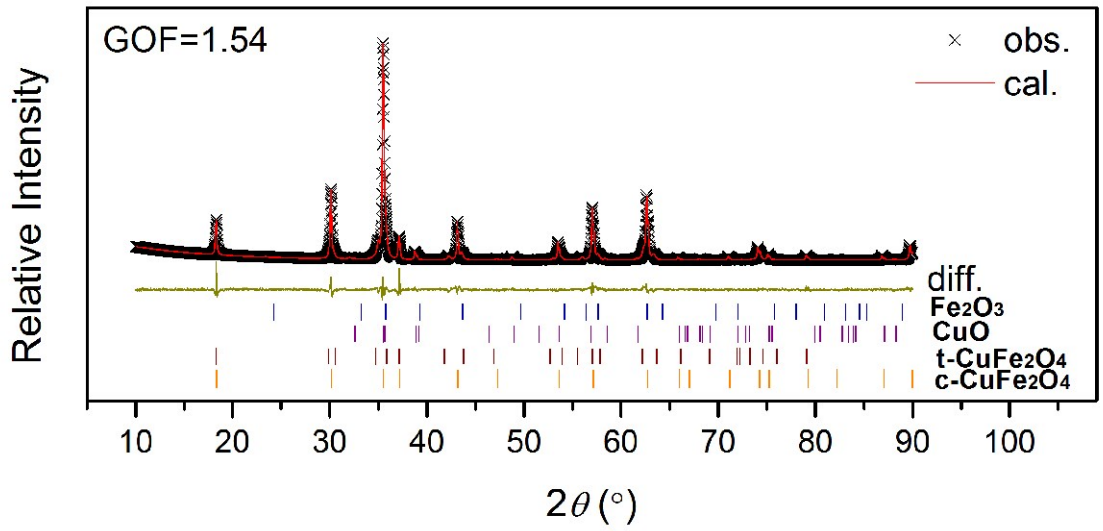

Figure S8. Rietveld refinement result for the product sintered at 1000 °C for 3 h from Fe_2O_3 precursor and CuO. The scanned value (obs.), the refined value (cal.) and the difference (diff) are indicated. The standard XRD patterns retrieved from the ICDD database include t-$CuFe_2O_4$ (PDF#34-0425), c-$CuFe_2O_4$ (PDF#77-0010), CuO (PDF#80-1268), and hematite (α-Fe_2O_3, PDF#85-0599). The goodness-of-fit of this refinement is 1.54.