Supplementary Information

Crystal Chemistry and Antibacterial Properties of Cuperiferous Hydroxyapatite

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SI 1:

PXRD Data of Undoped HA During Successive Sintering/Quenching Cycles within the Solid State Synthesis Route

As discussed in the main text, the preparation of single phase Cu-doped HA via the solid state synthesis route is only achieved after the 4th or 5th quenching cycle, as shown for case of sample HA2SS below. In contrast, a similar result is achieved after one only quench cycle when the wet chemical method is implemented. This is the primary evidence suggesting that the wet chemical approach is more time efficient approach for producing single phase Cu-doped HA systems.

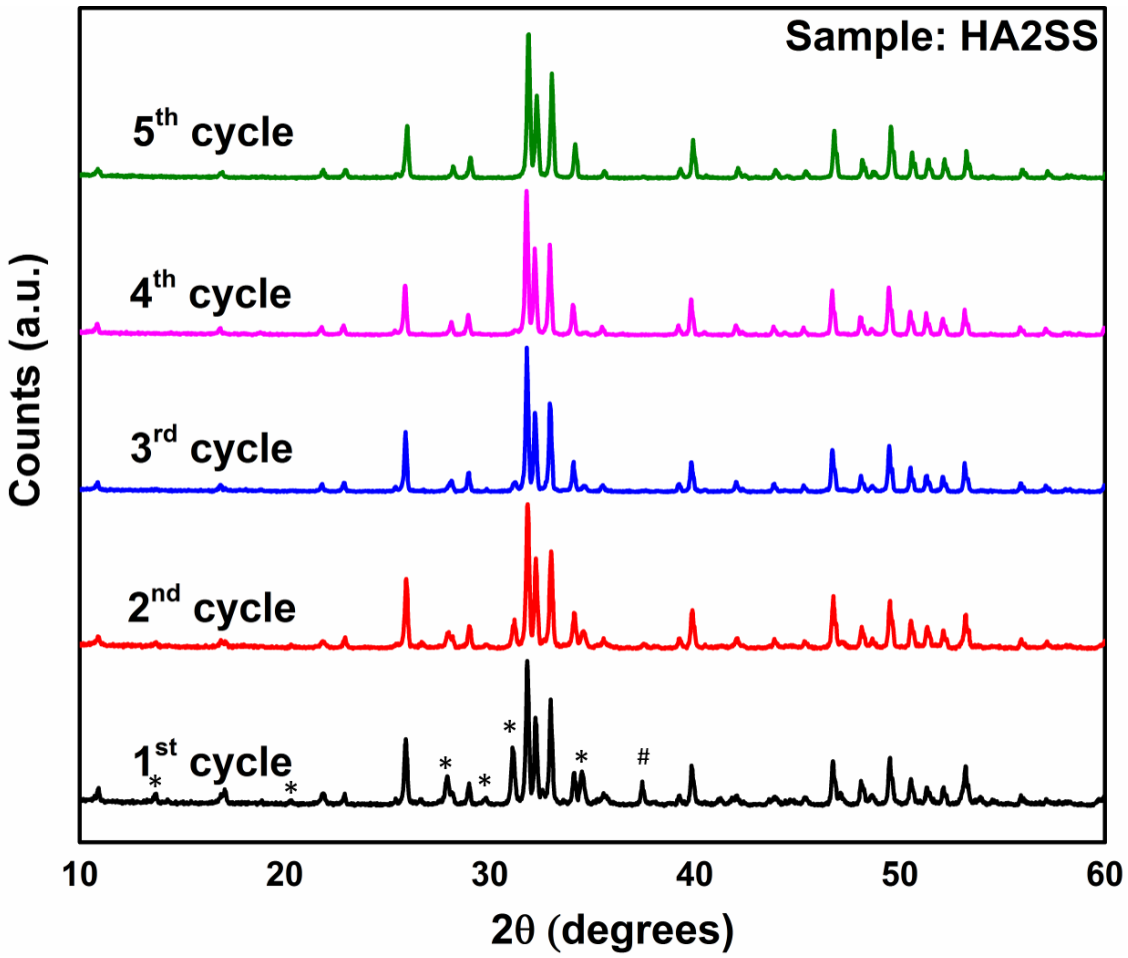

Figure SI1. PXRD data showing the phase composition of sample HA2SS after successive sintering/quench cycles. The impurities observed are β-$Ca_3(PO_4)_2$ (β-TCP, identified with *) and CaO (identified with #).

SI 2:

FESEM Images of the Cu-Doped HA Biomaterials Produced via the Wet Chemical Synthetic Route

As discussed in the main text, a particle size <500 nm is observed from the FESEM images of the samples produced via the wet chemical route. This smaller particle size of wet chemical route samples is suggested to be the main reason that these samples show an improved antibacterial efficacy compared to the solid state prepared samples.

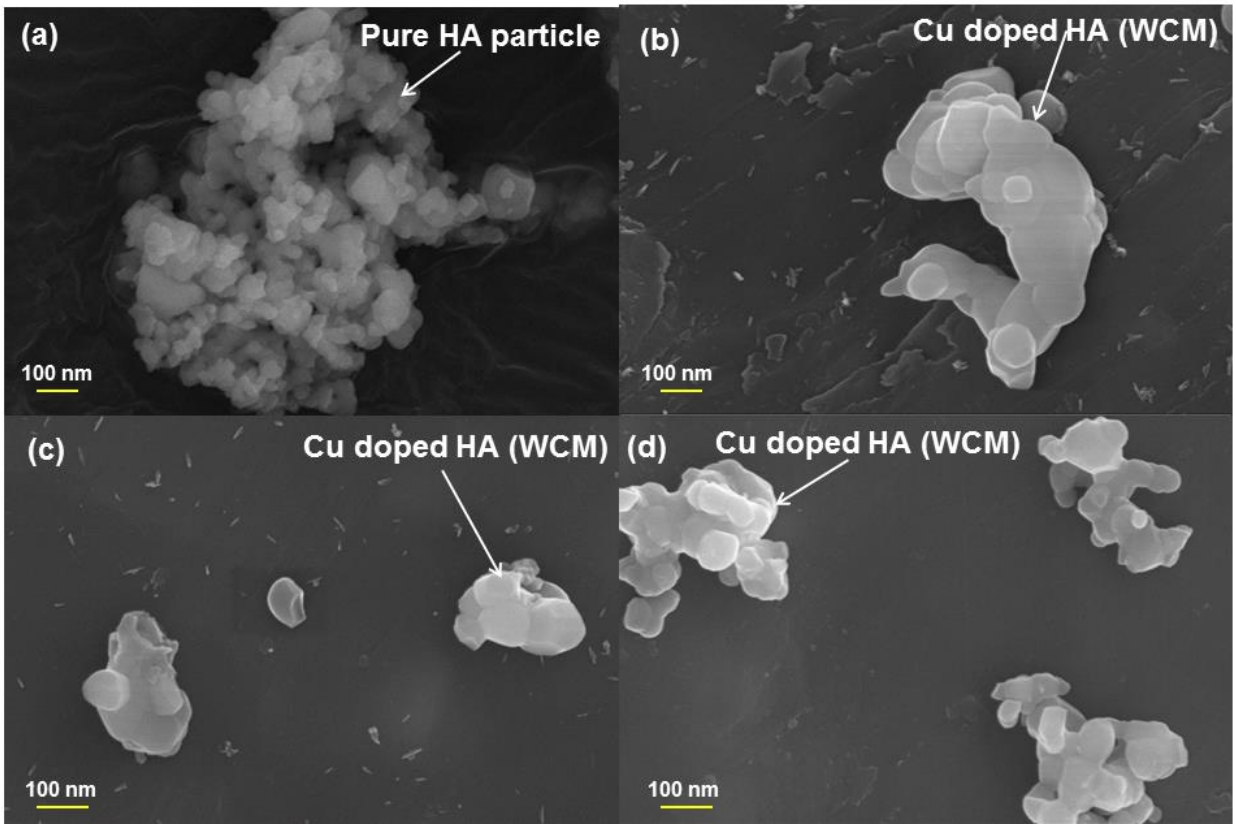

Figure SI2. FESEM images of samples (a) HAWCM, (b) HA2WCM, (c) HA6WCM and (d) HA8WCM synthesized via the wet chemical route.

SI 3:

PXRD of Slow Cooled HA Sample HA6SS1 (x = 0.6)

In the main text the XANES data shown in Figure 7 shows a predominant presence of the Cu^{2+} oxidation state for slow cooled x = 0.6 sample HA6SS1, in comparison to the air quenched analogues HA6SS and HA6WCM. This can be further supported by the XRD data analysis of HA6SS1, which exhibits the presence of CuO at the ~2 - 3% level.

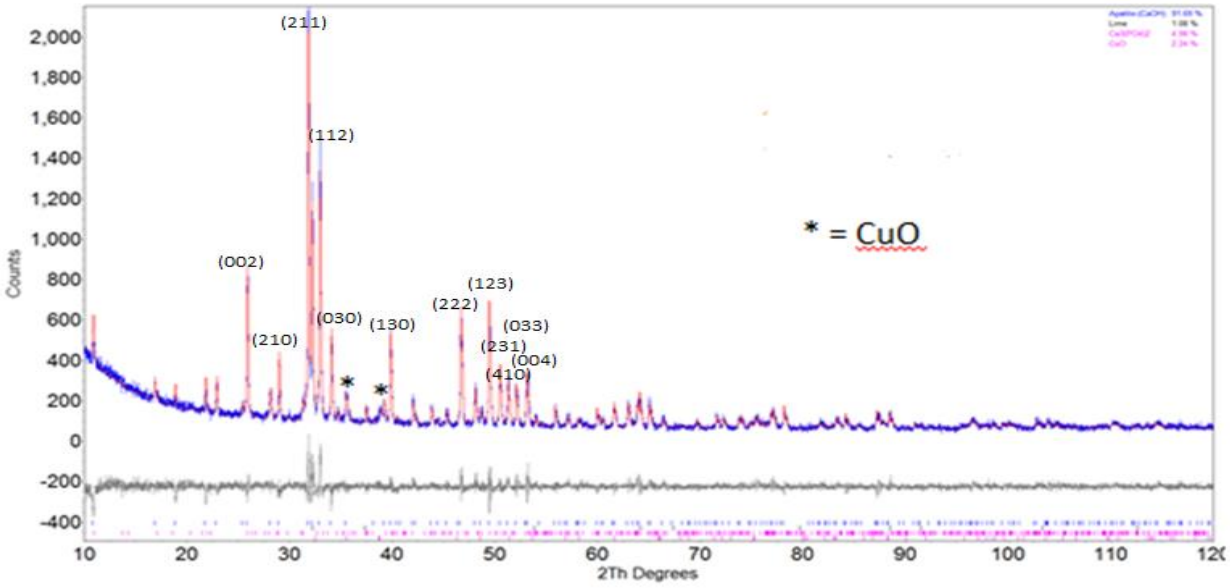

Figure SI3. Phase composition of HA6SS1 (slow cooled from 1100°C) indicating the presence of a secondary CuO phase.

SI 4:

EXAFS Data of Quenched and Non-Quenched Samples

As discussed in the main text, the EXAFS data of quenched and non-quenched samples prepared via the solid state and wet chemical routes is presented in SI 4. These first shell EXAFS fittings were used to determine the Cu-O distances in the respective samples.

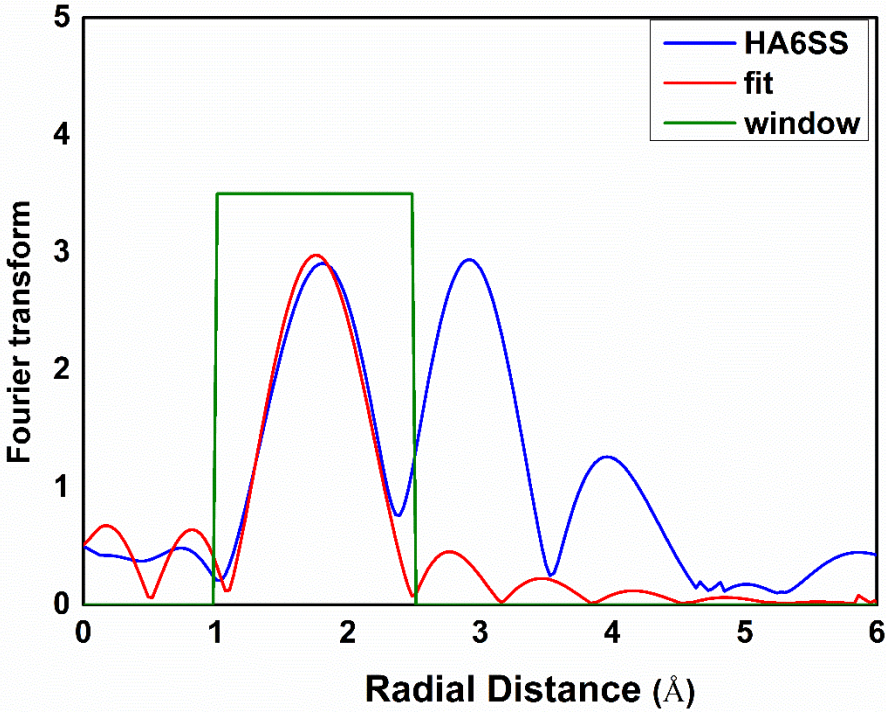

Figure SI4(a). 1st shell EXAFS data of quenched sample obtained from the solid state reaction route (HA6SS).

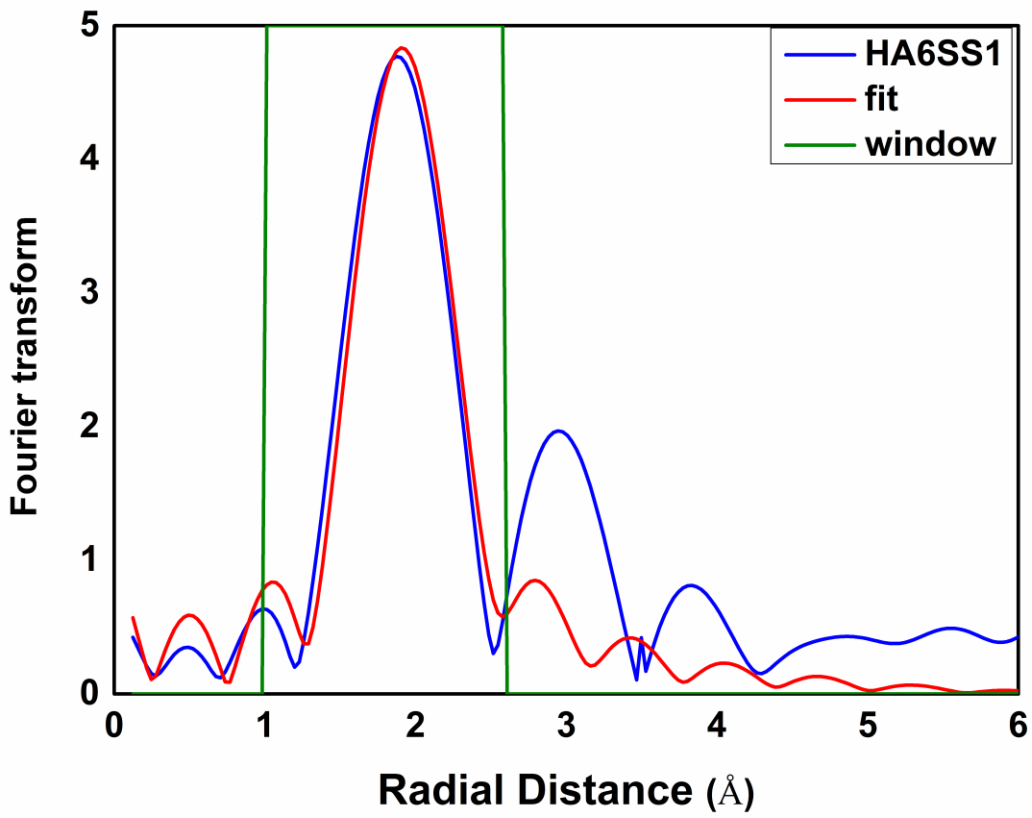

Figure SI4(b). 1st shell EXAFS fitting of the non-quenched (slow cooled) sample from the solid state reaction route (HA6SS1).

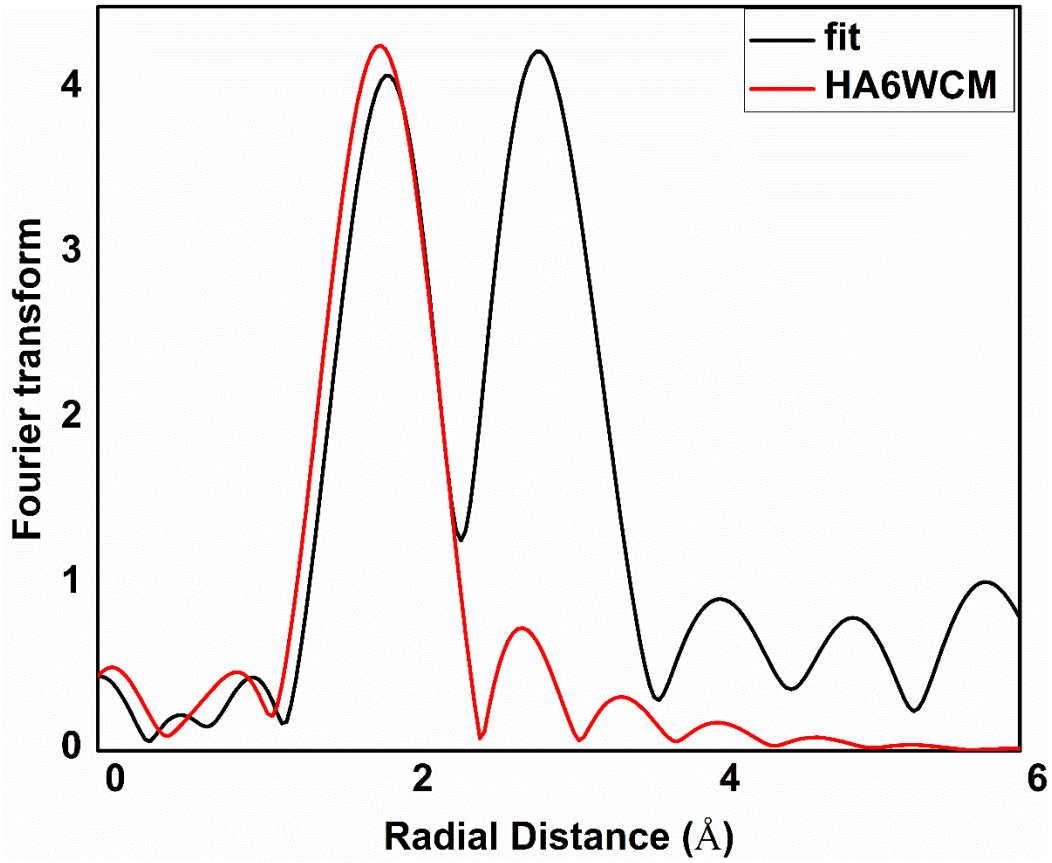

Figure SI4(c). 1st shell EXAFS fitting of the quenched sample obtained from wet chemical reaction route (HA6WCM).