Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Size-and Phase-Dependent Structure of Copper (II) Oxide Nanoparticles

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I. Potential energy profiles for a 4 nm particle

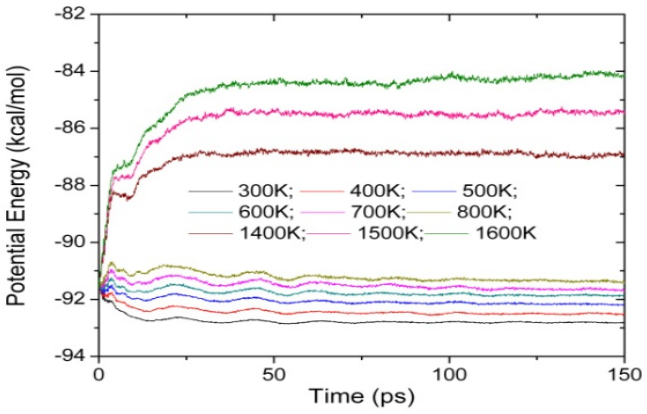

Figure S1. Potential energy profiles of a 4nm particle as a function of time at different temperatures.

II. Melting point empirical model

We used the model proposed by Jiang and Shi[1] to calculate the melting temperature as a function of nanoparticle size, $T_m(r)$ using the relation:

$$\frac{T_m(r)}{T_m(\infty)} = exp\left[(1-\alpha)/\left(\frac{r}{r_0}-1\right)\right] \quad (1)$$

where $T_m(\infty)$ is the bulk melting point of CuO (1600 K), $r_0$is minimum radius and α is material specific constant.

$$r_0 = (3 - d)h$$

where the $d = 0$ for spherical nanoparticles and h is the atomic diameter of CuO (0.6845 nm).[2,3] The constant α is calculated using the equation:

$$\alpha = \frac{2S_{vib}}{3R} + 1$$

where$S_{vib}(\infty) = 7.016$ J/mol.K^3 is the bulk melting entropy and R = 8.31 J/mol.K is the ideal gas constant. This method has been used extensively for the prediction of size-dependent thermophysical properties of many different nanoparticles including metal oxides.[4,5]It should be noted that Equation (1) is valid for nanoparticles of radii $r \geq 2r_0 \approx 3h$.[1]

III. XRD temperature dependence

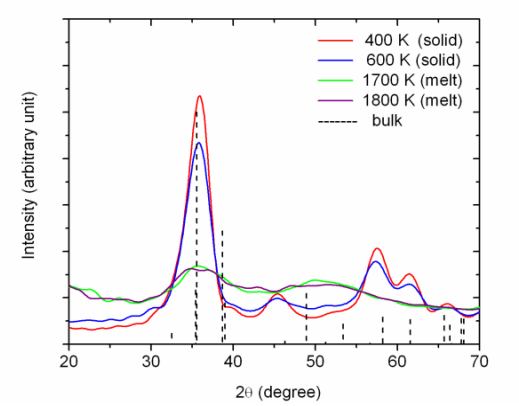

Figure S2. XRD profiles of CuO nanoparticles of diameter 4 nm at different temperatures.

References

1 Z. Zhang, X. X. Lu and Q. Jiang, *Phys. B*, 1999, **270**, 249–254.

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4 P. A. Bhatt, A. Pratap and P. K. Jha, *J. Therm Anal Calorim*, 2012, **110**, 535–538.

5 S. Mishra, S. K. Gupta, P. K. Jha and A. Pratap, *Mater. Chem. Phys.*, 2010, **123**, 791–794.