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:

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

(1)
where $T_m(\infty)$ is the bulk melting point of CuO (1600 K), $r_0$ is minimum radius and $\alpha$ 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).\textsuperscript{2,3} The constant $\alpha$ is calculated using the equation:

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

where $S_{\text{vib}}(\infty) = 7.016$ J/mol.K\textsuperscript{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.\textsuperscript{4,5} It should be noted that Equation (1) is valid for nanoparticles of radii $r \geq 2r_0 \approx 3h$.\textsuperscript{1}

### III. XRD temperature dependence

![XRD profiles of CuO nanoparticles of diameter 4 nm at different temperatures.](image)

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

### References