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P-type Cu_7Te_5 Single-crystalline Nanocuboids: Size-Controlled Synthesis and Their Large-scale Self-assembly

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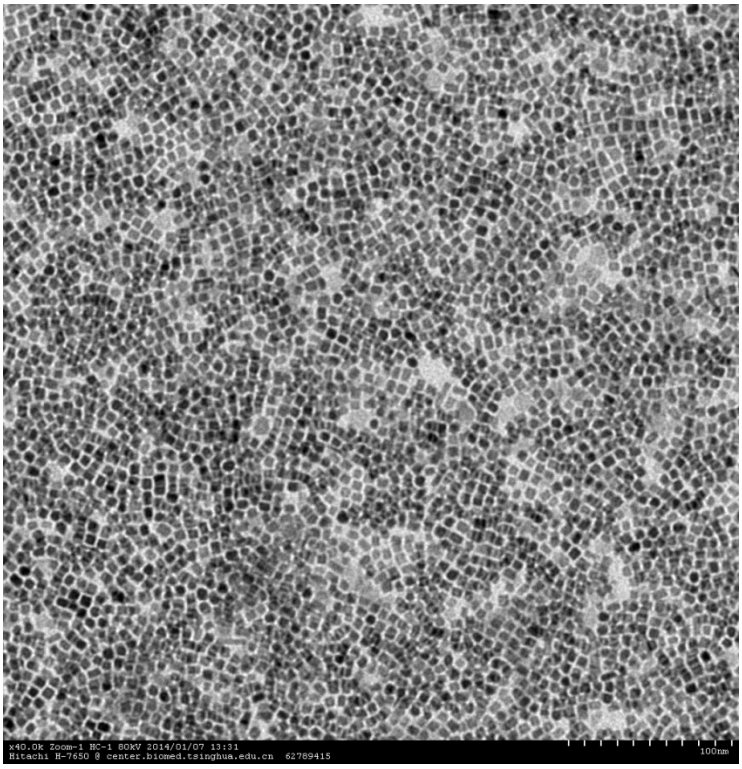
Supporting Information:



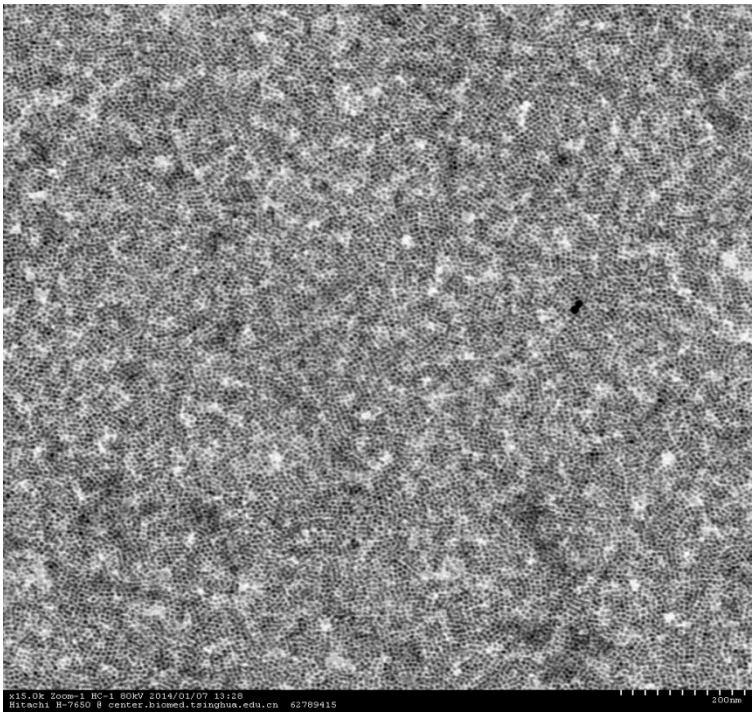


Figure S1 Large-scale TEM images of as-prepared Cu_7Te_5 nanocuboids.

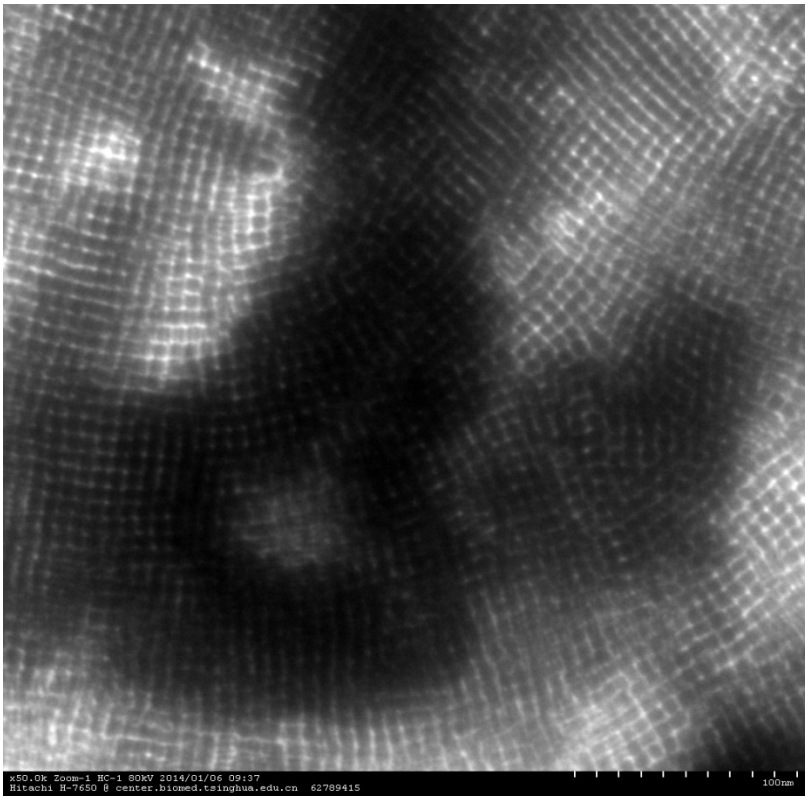


Figure S2 TEM image of large-scale self-assembly.

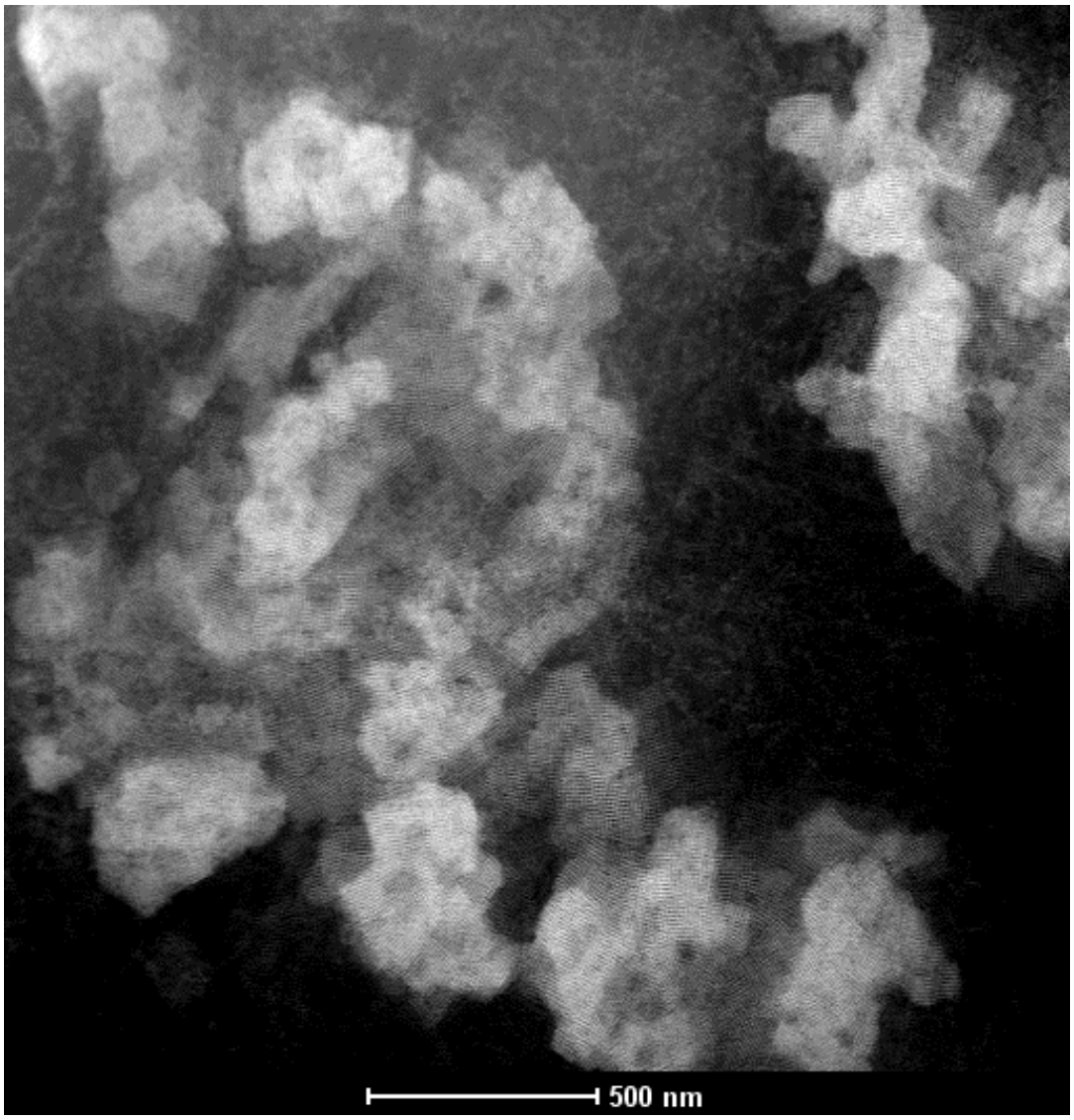


Figure S3 STEM image of large-scale micrometer sized superstructures composed by nanocube-liked nanocuboids.

The analysis of the largest exposed faces of the crystal:

As shown in Fig. 1, for the Cu_7Te_5 nanocuboids, the distance measured between two adjacent fringes is 0.70 nm and 0.52 nm, which is the interfacial spacing of the orthorhombic Cu_7Te_5 (0 0 2) and (0 3 2), and the corresponding fast Fourier transform (FFT) pattern contains the diffraction spots from the (0 3 2) and (0 3 0) planes of orthorhombic phase Cu_7Te_5.

According to Zone law, the following equation exists between the zone axis [*u v w*] and the indices of crystal face *(h k l)* belongs to the zone axis[1]

$$hu + kv + lw = 0,$$

So, if we know two planes (h_1 k_1 l_1) and (h_2 k_2 l_2) which did not parallel, we can get the zone axis by using the following equation:

$$u{:}v{:}w = \begin{bmatrix} k1 & l1 \\ k2 & l2 \end{bmatrix}{:}\begin{bmatrix} l1 & h1 \\ l2 & h2 \end{bmatrix}{:}\begin{bmatrix} h1 & k1 \\ h2 & k2 \end{bmatrix}.$$

So according to plane (0 3 2) and plane (0 3 0), we can calculate the zone axis, which is [1 0 0]. Last but not least, we can know the largest exposed faces of the crystal belong to high-indexed {1 0 0} planes.[2]

References:

1. G. X. Hu, X. Cai, Y. H. Rong, *Fundamentals of Materials Science*, 2nd Ed., China, Shanghai Jiao Tong University Press Co., Ltd, 2006, 19-35.
2. F. R. Zhou, P. L. Zhu, X. Z. Fu, R. Q. Chen, R. Sun and C. P. Wong, *CrystEngComm*, 2014, **16**, 766-774.