

Supplementary Information

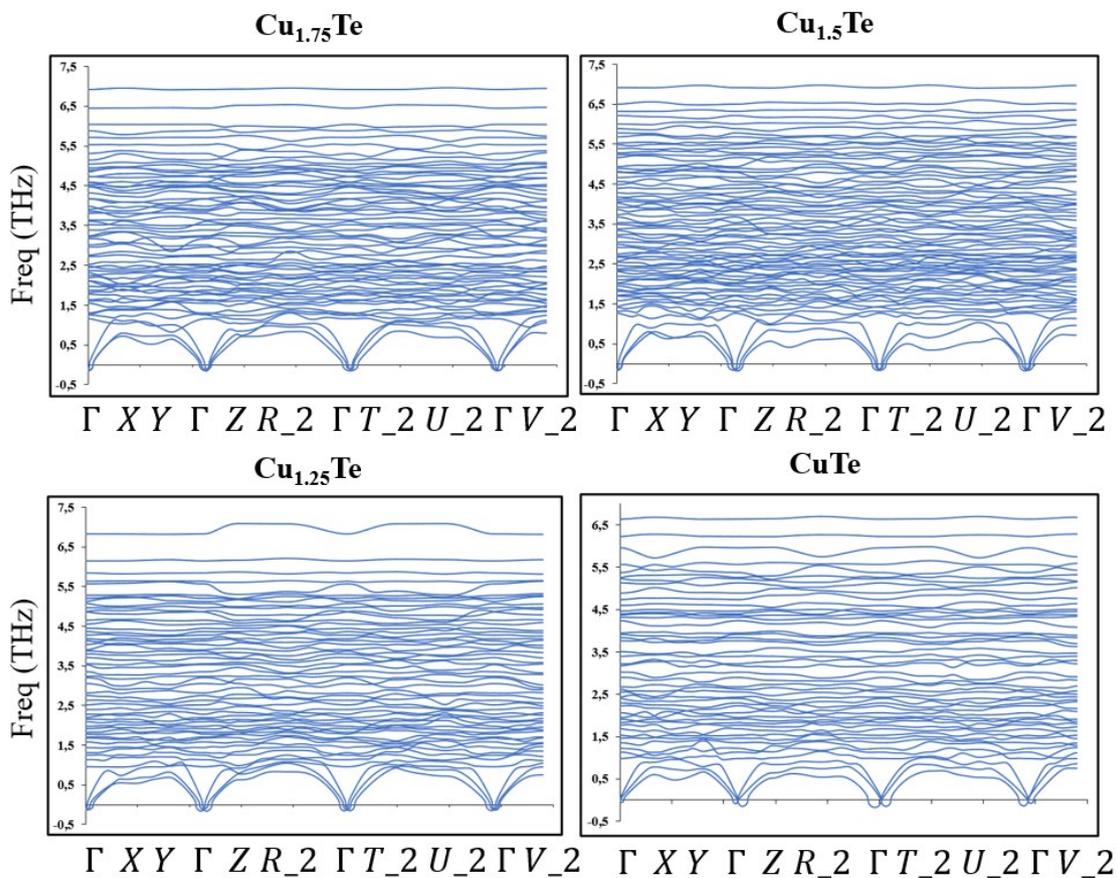


Figure S1. Phonon dispersion of copper telluride NCs for Cu/Te ratios: 1.75, 1.5, 1.25 and 1.

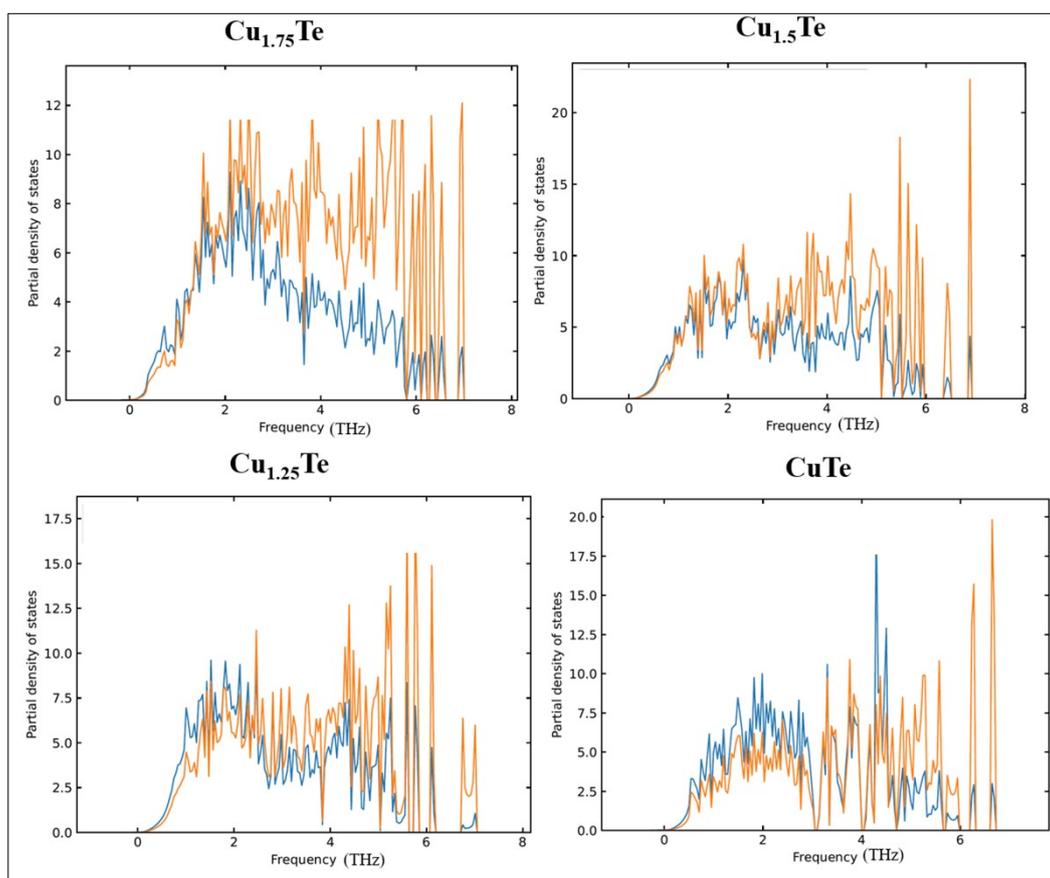


Figure S2. Partial vibrational density of states of copper telluride NCs for Cu/Te ratios: 1.75, 1.5, 1.25 and 1. Orange and blue graphs correspond to Cu and Te displacements, respectively.

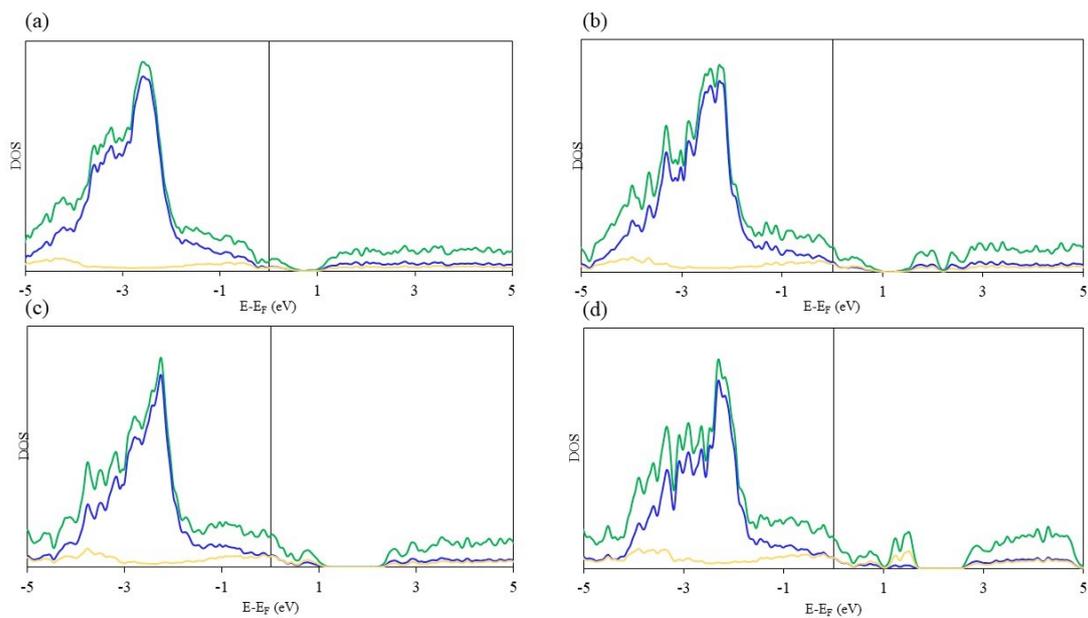


Figure S3. Total (DOS) and partial density of states (PDOS) for $\text{Cu}_{1.75}\text{Te}$ (a), $\text{Cu}_{1.5}\text{Te}$ (b), $\text{Cu}_{1.25}\text{Te}$ (c) and CuTe (d) NPs. Green graphs correspond to DOS, blue graphs to Cu PDOS and yellow graphs to Te PDOS.

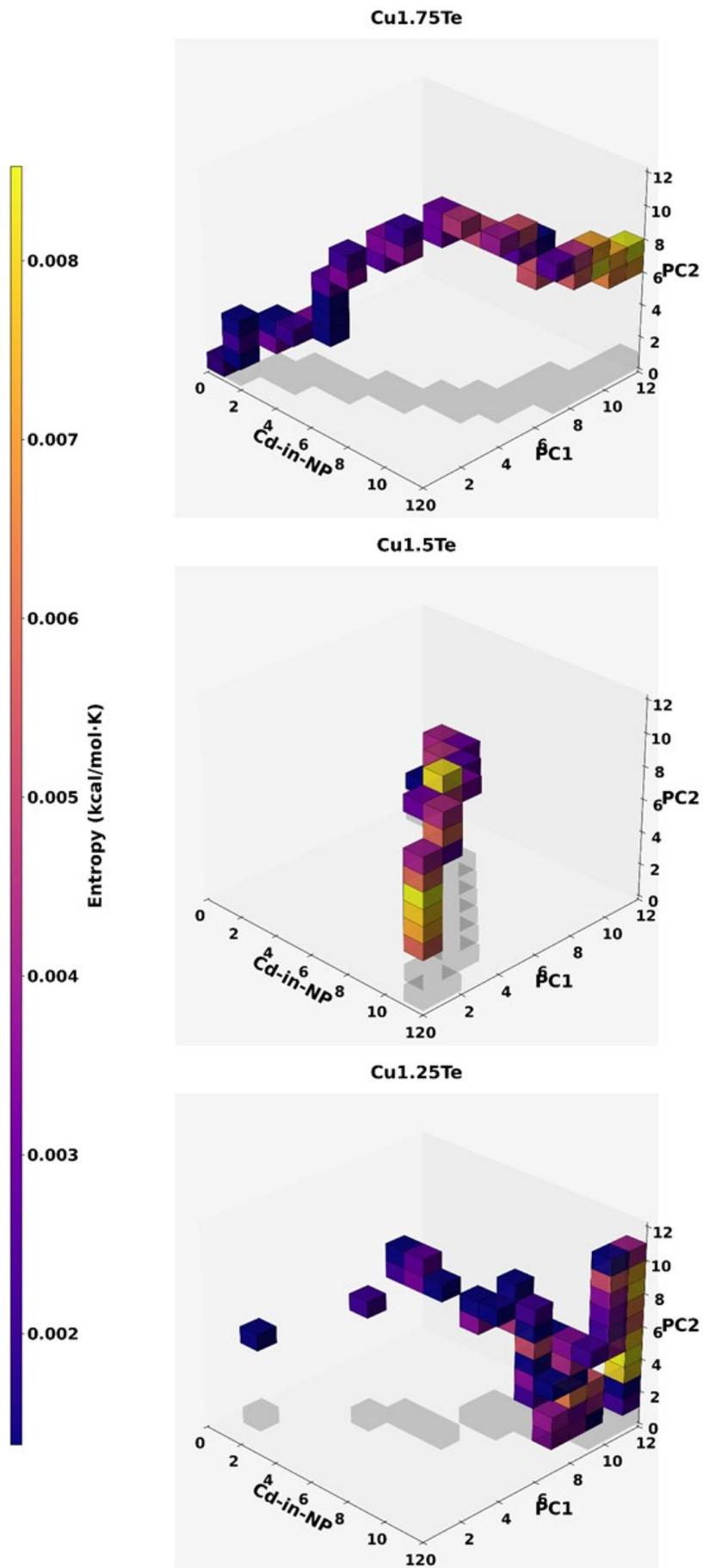


Figure S4. 3D voxel entropy plots for $\text{Cu}_{1.75}\text{Te}$ (top), $\text{Cu}_{1.5}\text{Te}$ (middle) and $\text{Cu}_{1.25}\text{Te}$ (bottom) NPs. PC1 is the direction in space that captures the most variance for the exchange trajectory (the dominating shape/structure mode). PC2 is the direction that explains the second-most proportion of the total variance. Cubes are colored according to the configurational entropy (see text for details). Bright colors (white/yellow/orange) correspond to high entropy (more diverse) configurations.

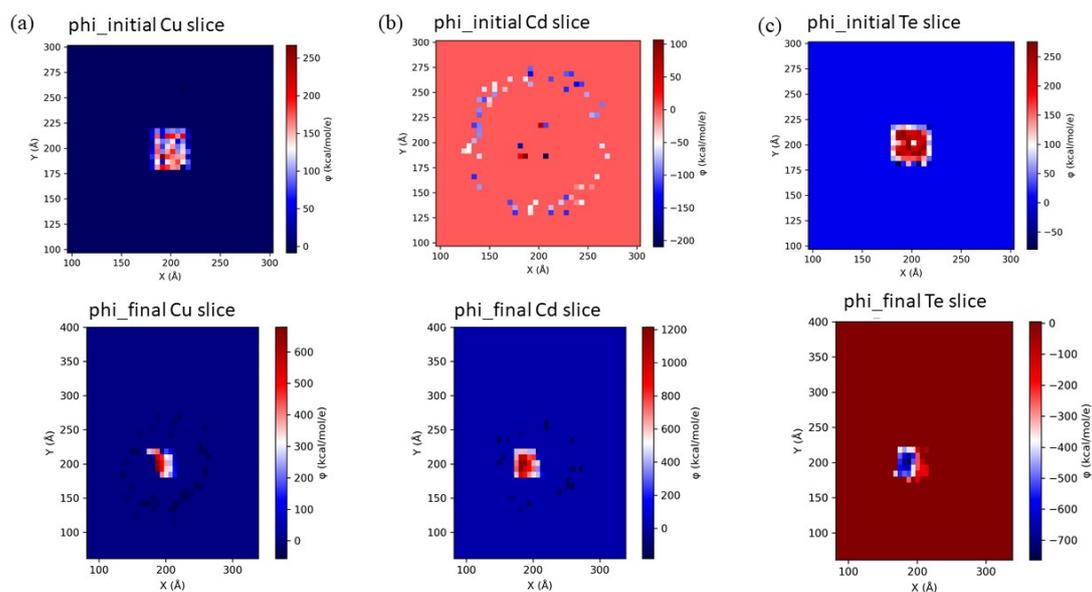


Figure S5. 2D slice plots of electrostatic potential (ϕ) for Cu, Cd and Te, in the $\text{Cu}_{1.75}\text{Te}$ NP.

Table S1. PCA weights for Cu_{1.75}Te NP.

Descriptor	PC1 weight	PC2 weight
volume	0.4938	-0.1335
aspect_ratio	0.4513	-0.1722
shape_ratio	-0.3504	0.7525
cd_te coordination number	0.4637	0.4430
cu_te coordination number	-0.4633	-0.4359

Table S2. PCA weights for Cu_{1.5}Te NP.

Descriptor	PC1 weight	PC2 weight
volume	-0.4247	-0.4864
aspect_ratio	0.0060	0.8418
shape_ratio	-0.5174	0.1429
cd_te coordination number	-0.5245	0.1337
cu_te coordination number	0.5261	-0.1284

Table S3. PCA weights for Cu_{1.25}Te NP.

Descriptor	PC1 weight	PC2 weight
volume	-0.5312	-0.2826
aspect_ratio	-0.1766	0.5989
shape_ratio	0.0295	0.7450
cd_te coordination number	0.5859	-0.0550
cu_te coordination number	-0.5852	0.0583