Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

A simple large-scale preparation and crystal phase control method of Cu_2Se by exfoliating from copper foam under Se-rich airflow

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Text S1: Calculation detail

In this work, ab initio molecular dynamics (AIMD) was used to perform theoretical simulations and combined with molecular dynamics to calculate the material properties at high temperatures. Since high temperatures will cause thermal vibrations of the atoms, the calculations for the material are accompanied by thermal rise and fall. Therefore, we calculated 10000 steps for the Cu_2Se cell after expanding 2 times all three directions of a_1, a_2, and a_3, and obtained 10000 instantaneous structures and the corresponding lattice constants a_1, a_2, and a_3, then the average values were calculated to obtain the corresponding calculation results.

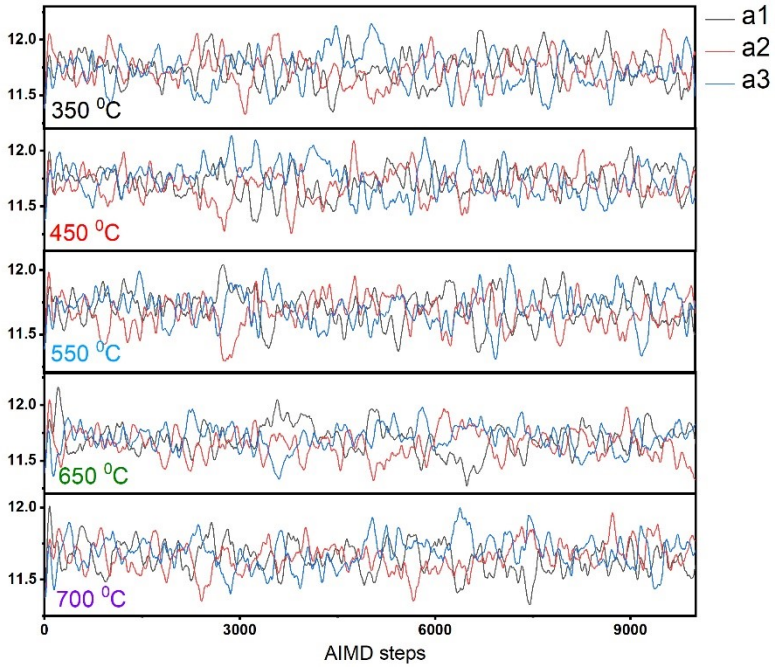

Fig. S1 Calculated lattice constants a_1, a_2, a_3 for Cu_2Se at 350 ^{0}C, 450 ^{0}C, 550 ^{0}C, 650 ^{0}C, 700 ^{0}C

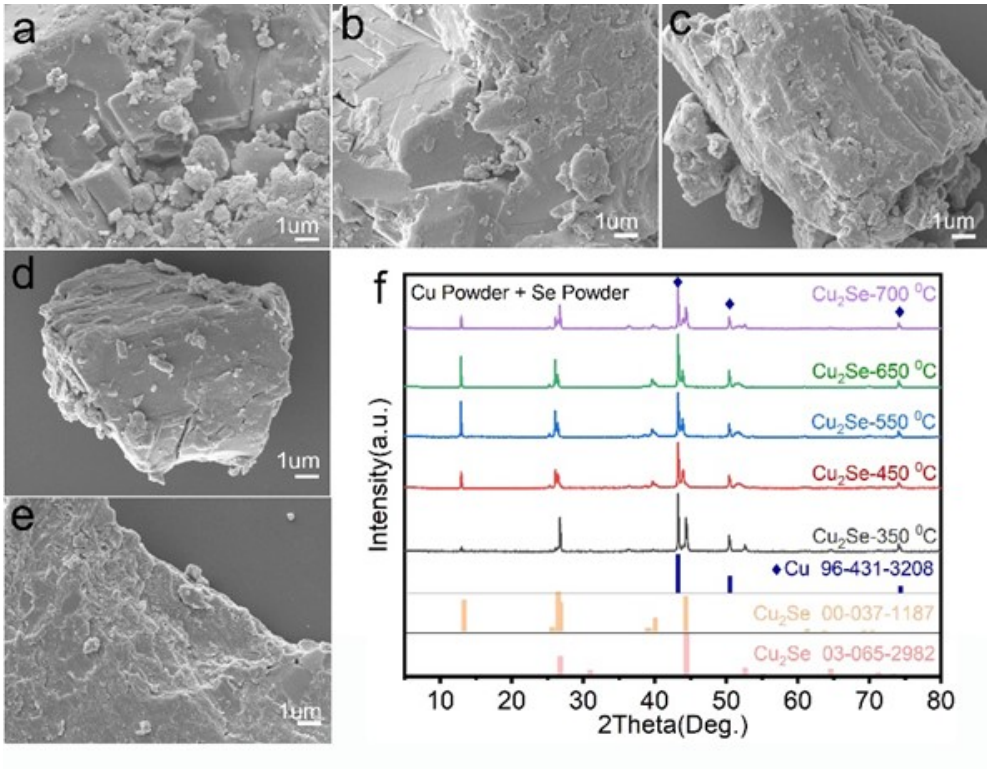

Fig S2. (a-e) Cu_2Se-GX (X=350 ^{0}C, 450 ^{0}C, 550 ^{0}C, 650 ^{0}C and 700 ^{0}C) prepared by calcination of copper and selenium powders after complete mixing, (f) XRD pattern of Cu_2Se-GX.

Table S1. Cu, Se content of Cu_2Se-550 ^{0}C

	ICP (%)	XPS (%)
Cu	62.6	22.4
Se	35.5	13.6