Synthesis, structure and properties of the layered oxyselenide $Ba_2CuO_2Cu_2Se_2$

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Table S1. Crystallographic parameters of $Ba_2CuO_2Cu_2Se_2$ refined from NPD pattern measured at room temperature. The occupancy rates were released during the refinement.

Phase data						
Formula: $Ba_2CuO_2Cu_2Se_2$						
Space group: *I*4/*mmm* (No.139)						
a = 4.0884(1) (Å) *c*= 19.6882(7) (Å)						
R_{wp}: 5.2%, R_p: 4.3%, χ^2: 1.1						
Atomic parameters						
site	Wyck.	x	y	z	Occ.	100*Uiso
Cu(1)	4d	1/2	0	1/4	0.976(9)	1.68(7)
Cu(2)	2a	0	0	0	0.975(10)	0.78(8)
Ba	4e	1/2	1/2	0.0916(1)	1.008(10)	0.79(8)
Se	4e	0	0	0.17503(9)	1.000(8)	0.93(7)
O	4c	1/2	0	0	0.988(12)	1.26(9)

Table S2. Crystallographic parameters of $Ba_2CuO_2Cu_2Se_2$ refined from NPD pattern measured at 3K.

Phase data						
Formula: $Ba_2CuO_2Cu_2Se_2$						
Space group: *I*4/*mmm* (No.139)						
a = 4.0715 (1) (Å) c= 19.5964 (5) (Å)						
R_{wp}: 5.0%, R_p: 4.34%, $\chi 2$: 1.2						
Atomic parameters						
site	Wyck.	x	y	z	Occ.	100*Uiso
Cu(1)	4d	1/2	0	1/4	1	0.34(3)
Cu(2)	2a	0	0	0	1	0.32(4)
Ba	4e	1/2	1/2	0.0918(1)	1	0.11(5)
Se	4e	0	0	0.1753(1)	1	0.14(3)
O	4c	1/2	0	0	1	0.71(5)
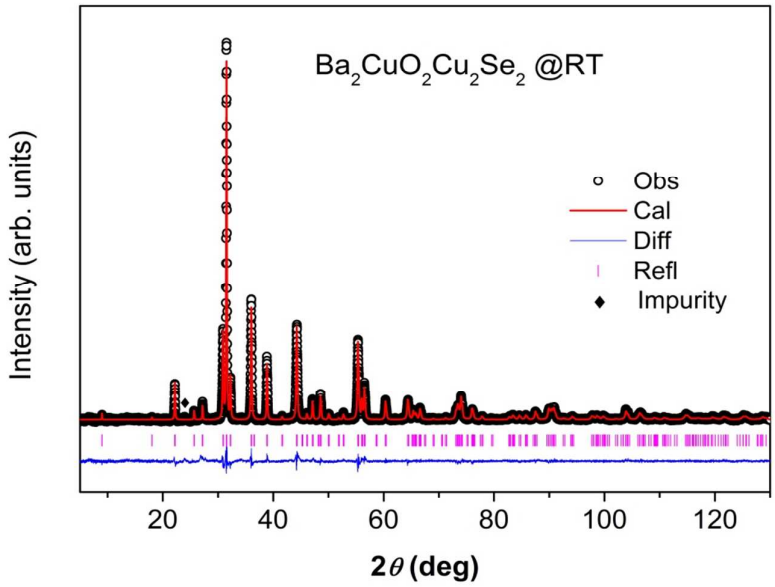
Fig. S1. The powder XRD diffraction data for $Ba_2CuO_2Cu_2Se_2$ at room temperature and the Rietveld refinement. Observed (black circle), calculated (red line), difference (blue line), and the allowed Bragg reflections (ticks) profiles are shown. A little unknown impurity is marked with black diamond symbol.