

Synthesis, crystal structure, photocatalysis, photocurrent response: one-dimensional $\text{K}_2\text{HgSnSe}_4$ and three-dimensional $\text{Na}_6\text{Cu}_8\text{Sn}_3\text{Se}_{13}$

Gele Teri,^a Na Li,^a Sagala Bai,^a Namila E,^a and Menghe Baiyin^{*a}

(College of Chemistry & Environmental Science, Inner Mongolia Normal University, Hohhot, Inner Mongolia 010022, P. R. China)

^{*a} E-mail: baiymh@imnu.edu.cn

Contents:

Table S1. Selected bond lengths [Å] and angles [°] for **1**.

Table S2. Selected bond lengths [Å] and angles [°] for **2**.

Figure S1. SEM-EDS analysis of compounds **1** and **2**.

Figure S2. Simulated and experimental power XRD patterns of compounds **1** and **2**.

Figure S3. UV-vis reflectance spectra of compounds **1** and **2**.

Figure S4. DTA analysis of compounds **1** and **2**.

Figure S5. Photoluminescence spectra of compounds **1** and **2**.

^{*a} Corresponding author.
E-mail address: baiymh@imnu.edu.cn.

Table S1 Selected bond lengths (Å) and angles (°) for compound K₂HgSnSe₄ (1)

Se1-Sn1 ⁴	2.620(5)	Se1 ⁴ -Hg1-Se1 ⁸	116.10(10)
Hg1-Se1 ¹¹	2.620(5)	Se1 ⁴ -Hg1-Se1	96.91(18)
Hg1-Se1 ⁸	2.620(5)	Se1 ⁸ -Hg1-Se1 ¹¹	116.09(10)
Hg2-Se1 ⁴	2.620(5)	Se1 ⁸ -Hg1-Hg1 ¹⁴	48.45(9)
Hg3-Hg1 ⁴	3.4751(4)	Se1 ⁴ -Hg1-Hg1 ¹⁴	131.54(9)
Hg4-Hg1 ¹⁴	3.4751(4)	Se1 ⁴ -Hg1-Hg1 ⁴	48.45(9)
Hg5-Se1 ¹¹	2.620(5)	Se1-Hg1-Hg1 ¹⁴	131.55(9)
Hg6-Se1 ⁸	2.620(5)	Se1-Hg1-Hg1 ⁴	48.46(9)
Hg7-Se1 ⁴	2.620(5)	Se1 ¹¹ -Hg1-Hg1 ⁴	131.55(9)
Hg1-Se1-Hg1 ⁴	83.09(18)	Se1 ¹¹ -Hg1-Hg1 ¹⁴	48.46(9)
Hg1-Se1-Sn1 ⁴	83.09(18)	Se1 ⁸ -Hg1-Hg1 ⁴	131.54(9)
Sn1-Se1-Hg1	0	Hg1 ⁴ -Hg1-Hg1 ¹⁴	180
Sn14-Se1-Hg1 ⁴	0	Se1 ⁴ -Sn1-Se1 ¹¹	116.09(10)
Sn1-Se1-Hg1 ⁴	83.09(18)	Se1 ⁸ -Sn1-Se1 ¹¹	96.91(18)
Sn1-Se1-Sn1 ⁴	83.09(18)	Se1-Sn1-Se1 ¹¹	116.09(10)
Se1 ⁴ -Hg1-Se1 ¹¹	116.09(10)	Se1 ⁴ -Sn1-Se1 ⁸	116.10(10)
Se1 ⁸ -Hg1-Se1 ¹¹	96.91(18)	Se1 ⁴ -Sn1-Se1	96.91(18)
Se1-Hg1-Se1 ¹¹	116.09(10)	Se1 ⁸ -Sn1-Se1	116.09(10)

Table S2 Selected bond lengths (Å) and angles (°) for compound Na₆Cu₈Sn₃Se₁₃ (2)

Sn01-Se03	2.5392(13)	Se03 ¹⁰ -Cu04-Cu04 ⁹	106.19(4)
Sn01-Se03 ¹	2.5392(13)	Se03 ¹⁰ -Cu04-Cu04 ³	52.37(5)
Sn01-Se03 ²	2.5392(13)	Se03-Cu04-Cu04 ⁹	137.84(4)
Sn01-Se03 ³	2.5392(13)	Cu04 ⁹ -Cu04-Cu04 ³	90.003(1)
Se02-Cu04	2.555(2)	Cu04 ⁹ -Cu04-Cu04 ⁴	90.003(1)
Se02-Cu04 ⁴	2.555(2)	Cu04 ³ -Cu04-Cu04 ⁴	90
Se02-Cu04 ⁵	2.555(2)	Se03-Sn01-Se03 ¹	106.50(3)
Se02-Cu04 ³	2.555(2)	Se03 ¹ -Sn01-Se03 ²	115.60(6)
Se02-Cu04 ⁶	2.555(2)	Se03-Sn01-Se03 ²	106.50(3)
Se02-Cu04 ⁷	2.555(2)	Se03 ¹ -Sn01-Se03 ³	106.50(3)
Se02-Cu04 ⁸	2.555(2)	Se03-Sn01-Se03 ³	115.60(6)
Se02-Cu04 ⁹	2.555(2)	Se03 ² -Sn01-Se03 ³	106.50(3)
Se03-Cu04 ⁹	2.4157(11)	Cu04 ³ -Se02-Cu04 ⁴	109.5
Se03-Cu04 ⁹	2.4158(11)	Cu04-Se02-Cu04 ⁴	70.5
Cu04-Cu04 ⁶	2.950(3)	Cu04 ⁵ -Se02-Cu04 ⁶	70.5
Cu04-Cu04 ³	2.950(3)	Cu04 ⁷ -Se02-Cu04 ⁸	109.5
Cu04-Cu04 ⁹	2.950(3)	Cu04 ⁷ -Se02-Cu04 ⁴	70.5
Cu04-Se02-Cu04 ⁷	109.5	Cu04 ⁵ -Se02-Cu04 ⁸	70.5
Cu04 ⁹ -Se02-Cu04 ⁶	70.5	Cu04-Se02-Cu04 ⁸	109.5
Cu04 ⁶ -Se02-Cu04 ⁸	109.5	Cu04 ⁵ -Se02-Cu04 ⁴	109.5
Cu04-Se03-Sn01	99.15(4)	Cu04 ⁵ -Se02-Cu04 ³	109.5

Cu04 ⁴ -Se03-Sn01	99.15(4)	Cu04 ³ -Se02-Cu04 ⁶	70.5
Cu04 ⁴ -Se03-Cu04	75.27(11)	Cu04 ⁹ -Se02-Cu04 ⁷	180.00(5)
Se02-Cu04-Cu04 ⁹	54.7	Cu04 ⁷ -Se02-Cu04 ⁶	109.5
Se02-Cu04-Cu04 ³	54.7	Cu04-Se02-Cu04 ⁵	180
Se02-Cu04-Cu04 ⁴	54.7	Cu04 ⁹ -Se02-Cu04 ⁸	70.5
Se03 ¹⁰ -Cu04-Se02	103.68(6)	Cu04 ⁹ -Se02-Cu04 ⁵	109.5
Se03 ¹¹ -Cu04-Se02	103.68(6)	Cu04 ⁹ -Se02-Cu04 ⁴	109.5
Se03-Cu04-Se02	103.68(6)	Cu04 ⁷ -Se02-Cu04 ⁵	70.5
Se03 ¹¹ -Cu04-Se03	114.59(4)	Cu04 ⁴ -Se02-Cu04 ⁸	70.5
Se03 ¹¹ -Cu04-Se03	114.59(4)	Cu04-Se02-Cu04 ³	70.5
Se03 ¹⁰ -Cu04-Se03	114.59(4)	Cu04 ⁶ -Se02-Cu04 ⁴	180.00(5)
Se03 ¹¹ -Cu04-Cu04 ³	137.84(4)	Cu04 ⁹ -Se02-Cu04 ³	109.5
Se03 ¹⁰ -Cu04-Cu04 ⁴	137.84(4)	Cu04-Se02-Cu04 ⁹	70.5
Se03-Cu04-Cu04 ³	106.19(4)	Cu04 ⁷ -Se02-Cu04 ³	70.5
Se03 ¹¹ -Cu04-Cu04 ⁴	106.19(4)	Cu04 ³ -Se02-Cu04 ⁸	180
Se03-Cu04-Cu04 ⁴	52.37(5)	Cu04-Se02-Cu04 ⁶	109.5
Se03 ¹¹ -Cu04-Cu04 ⁹	52.37(5)		

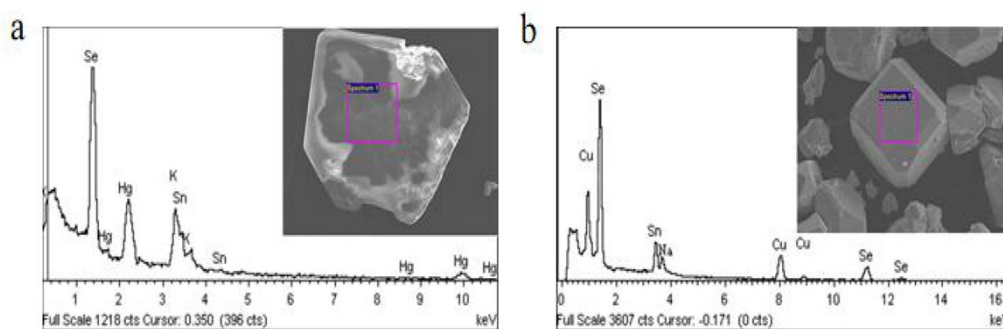


Figure S1. (a) SEM-EDS analysis of compound **1**; (b) SEM-EDS analysis of compound **2**.

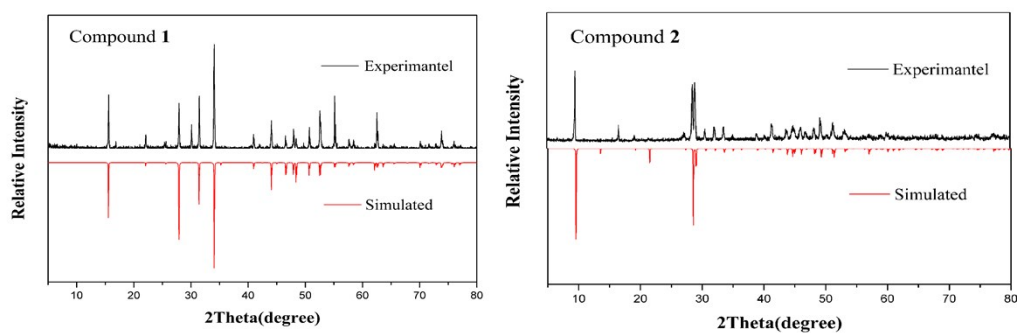


Figure S2. Simulated and experimental power XRD patterns of compounds **1** and **2**.

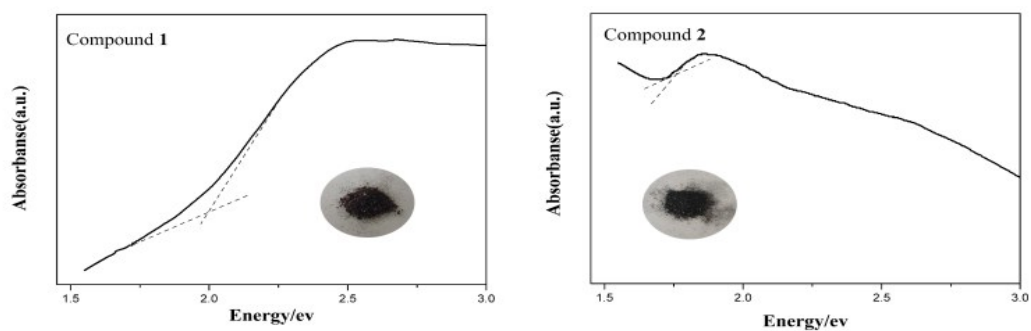


Figure S3. UV-vis reflectance spectra of compounds **1** and **2**.

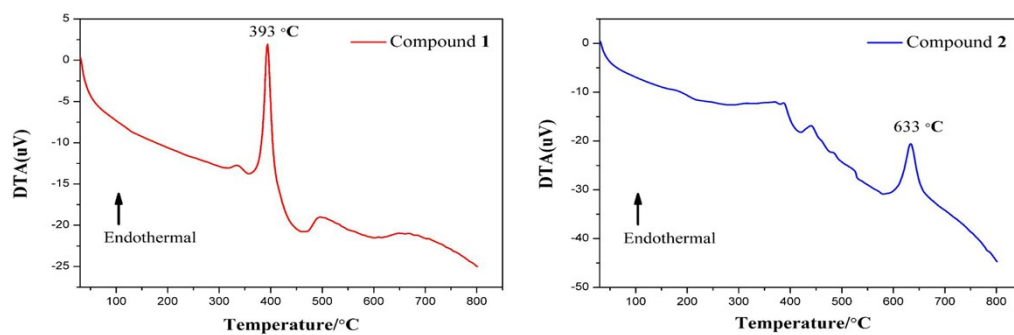


Figure S4. DTA analysis of compounds **1** and **2**.

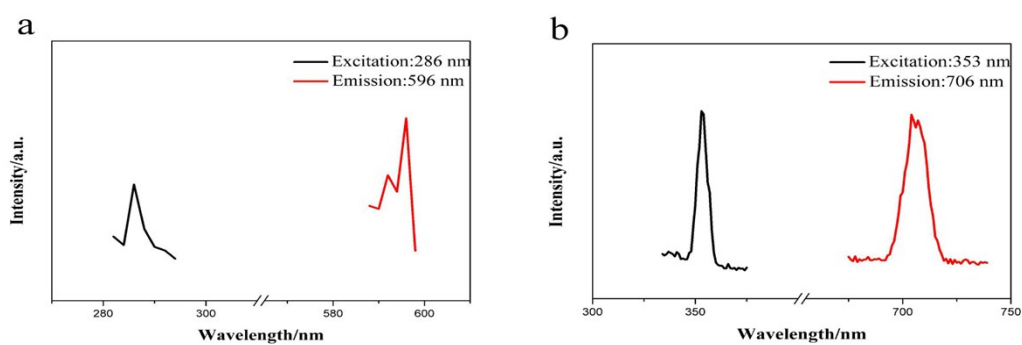


Figure S5. (a) Photoluminescence spectra of compound **1**;
(b) Photoluminescence spectra of compound **2**.