Supporting Information for

New Crystalline 1D/2D/3D Indium Selenides Directed by Piperidine and Auxiliary Solvents

Chaozhuang Xue,*a Jian Lin,^b Yifan Zhang,^a Zhiyang Liu,^a Rui Li,^a Shuwen Gong,*a and

Konggang Qu*a

^a School of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059,

China.

^b School of Materials Science and Engineering, Suzhou University of Science and Technology,

Suzhou 215009, China.



Fig. S1 SEM image and energy dispersive spectroscopy (EDS) of ISP-1.



Fig. S2 SEM image and energy dispersive spectroscopy (EDS) of ISP-2.



Fig. S3 SEM image and energy dispersive spectroscopy (EDS) of ISP-3.



Fig. S4 Powder X-ray diffraction (PXRD) patterns of unground ISP-1(a) and grinded ISP-1 (b).



Fig. S5 Powder X-ray diffraction (PXRD) patterns of ISP-2.



Fig. S6 Powder X-ray diffraction (PXRD) patterns of ISP-3.



Fig. S7 TGA curves of **ISP-1**, **ISP-2** and **ISP-3**. An abrupt weight loss between 150-400°C (200°C-300°C for **ISP-1**, 150°C-350°C for **ISP-2**, 250°C-370°C for **ISP-3**) is attributed to the carbonization of template as well as the loss of adsorbed auxiliary solvents. Obviously, the thermostability of ISP-3 is better than **ISP-1** and **ISP-2**, deduced from TGA curves.



Fig. S8 SEM image and energy dispersive spectroscopy (EDS) of ISP-4.



Fig. S9 Powder X-ray diffraction (PXRD) patterns of ISP-4.



Fig. S10 (a) 2D layered structure of **ISP-1** viewed from *b*-axis and (b) the stacked structure along with *b*-axis.



Fig. S11 Catenulate structures composed by four-membered rings in ISP-4.



Fig. S12 (a) Interlaced eight-membered ring constructed Channel A (along with *a*-axis) and (b) sixmember rings and four-member rings constructed channel B and C (along with *b*-axis) in **ISP-4**.

| Compounds | ISP-1 | ISP-2 | ISP-3 | ISP-4 |
|--------------------------------|----------------|----------------|----------------|----------------|
| Crystal system | Monoclinic | Monoclinic | Orthorhombic | Orthorhombic |
| Space group | P 21/c | P 21/c | Pbca | I b a m |
| Ζ | 4 | 2 | 8 | 16 |
| <i>a</i> (Å) | 11.949 (15) | 10.4695 (12) | 19.6419 (18) | 29.4109 (11) |
| <i>b</i> (Å) | 23.780 (3) | 14.4546 (15) | 19.642 (10) | 13.3976 (5) |
| <i>c</i> (Å) | 27.236 (3) | 7.2649 (8) | 33.131 (17) | 26.8483 (9) |
| α (deg.) | 90 | 90 | 90 | 90 |
| β (deg.) | 100.28 | 101.508 | 90 | 90 |
| γ (deg.) | 90 | 90 | 90 | 90 |
| $V(Å^3)$ | 7614.5 (16) | 1077.3 (2) | 12782 (9) | 10579.2 (6) |
| GOF on F^2 | 1.059 | 1.055 | 0.987 | 1.183 |
| $R_1, wR_2 (I > 2\sigma(I))^a$ | 0.0577, 0.1536 | 0.0919, 0.2261 | 0.0697, 0.1880 | 0.0300, 0.1087 |
| R_1 , wR_2 (all data) | 0.0858, 0.1761 | 0.1189, 0.2482 | 0.1421, 0.2265 | 0.0399, 0.1254 |

Table S1. Crystal data and structure refinement parameters for ISPs.

Note: ${}^{a}R_{1} = \sum ||F_{o}| - |F_{c}|| / \sum |F_{o}|, wR_{2} = [\sum w(F_{o}^{2} - F_{c}^{2})^{2} / \sum w(F_{o}^{2})^{2}]^{1/2}$

 Table S2. Elemental analysis results of ISPs.

| Elements (wt.) | N (%) | C (%) | H (%) |
|------------------------|-------|-------|-------|
| Calculated for ISP-1 | 3.21 | 13.75 | 2.77 |
| Experimental for ISP-1 | 3.48 | 14.33 | 3.31 |
| Calculated for ISP-2 | 3.20 | 13.72 | 2.76 |
| Experimental for ISP-2 | 3.15 | 13.26 | 3.34 |
| Calculated for ISP-3 | 2.72 | 11.67 | 2.35 |
| Experimental for ISP-3 | 2.64 | 12.05 | 2.57 |

Alert level B for crystallographic data of ISP-1 and ISP-2

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 7.34 eA-3 DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00 _refine_diff_density_min given = -5.111 Test value = -4.900

PLAT098_ALERT_2_B Large Reported Min. (Negative) Residual Density -5.11 eA-3

Response: Both Se and In atoms are heavy atoms and it is common for the large peaks appearing on the side of these heavy atoms. The large peaks near In and Se in ISP-1 and ISP-2 are derived from Fourier truncation error of heavy atom, resulting in Alert level B in checkcif.