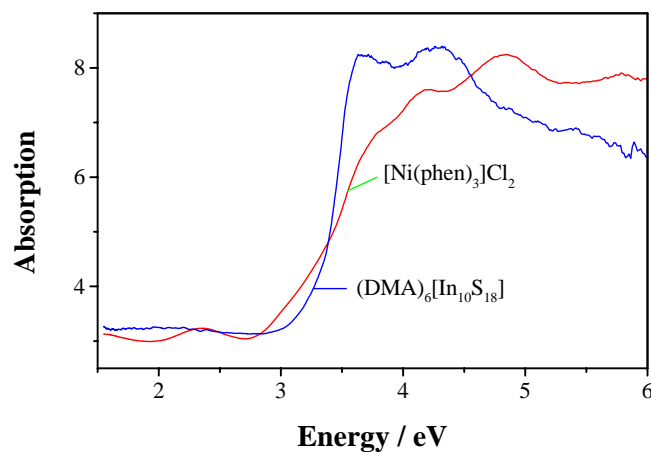


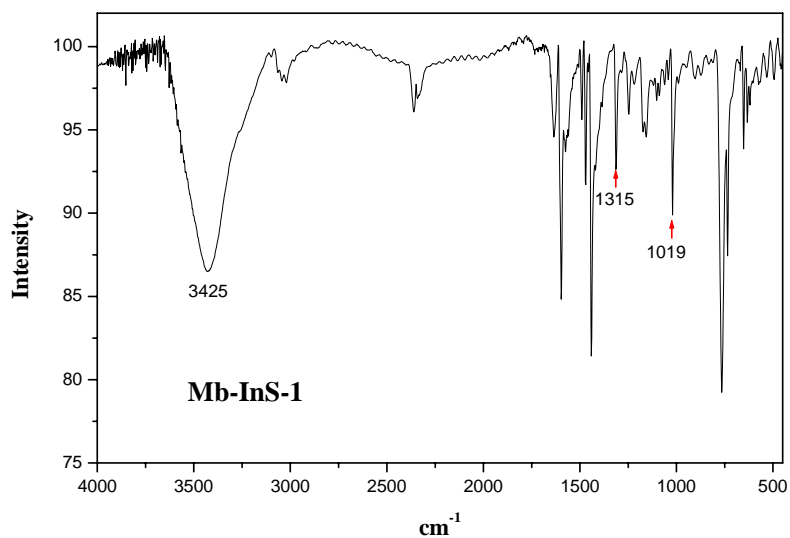
## Electronic Supplementary Information (ESI)

### Indium sulfide clusters integrated with 2,2'-bipyridine complexes

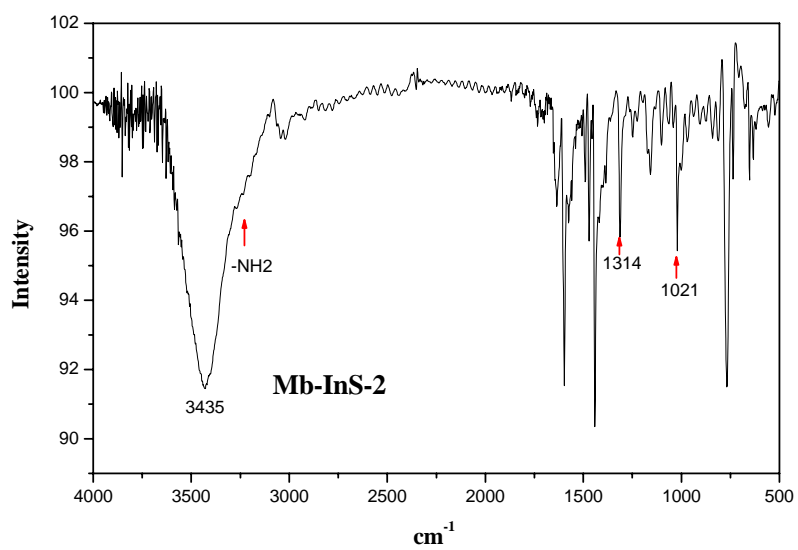
Ya-Ping Zhang,<sup>a</sup> Xu Zhang,<sup>a</sup> Wen-Qin Mu,<sup>a</sup> Wen Luo,<sup>a</sup> Guo-Qing Bian,<sup>a</sup> Qin-Yu Zhu<sup>\*a,b</sup> and Jie Dai<sup>\*a,b</sup>



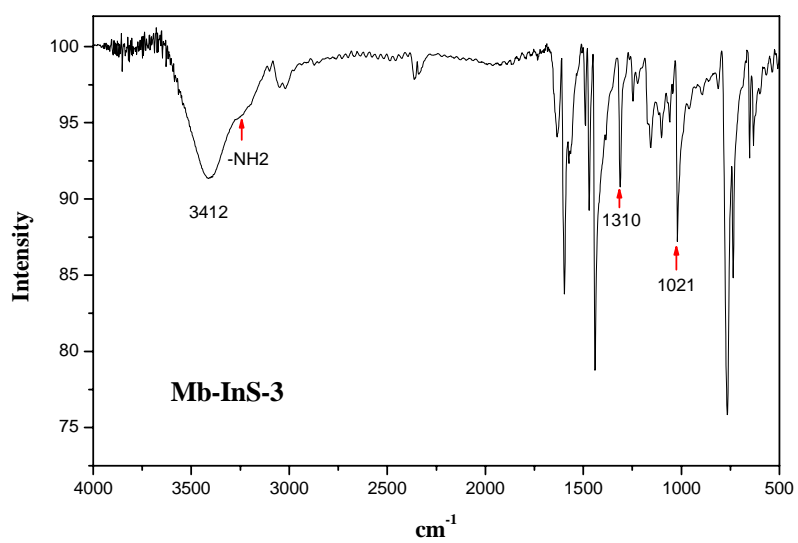
**SI-Fig.-1.** Electronic spectra of (HDMA)<sub>6</sub>In<sub>10</sub>S<sub>18</sub> (blue line) and [Ni(phen)<sub>3</sub>]Cl<sub>2</sub> (red line) in solid state.



(a)

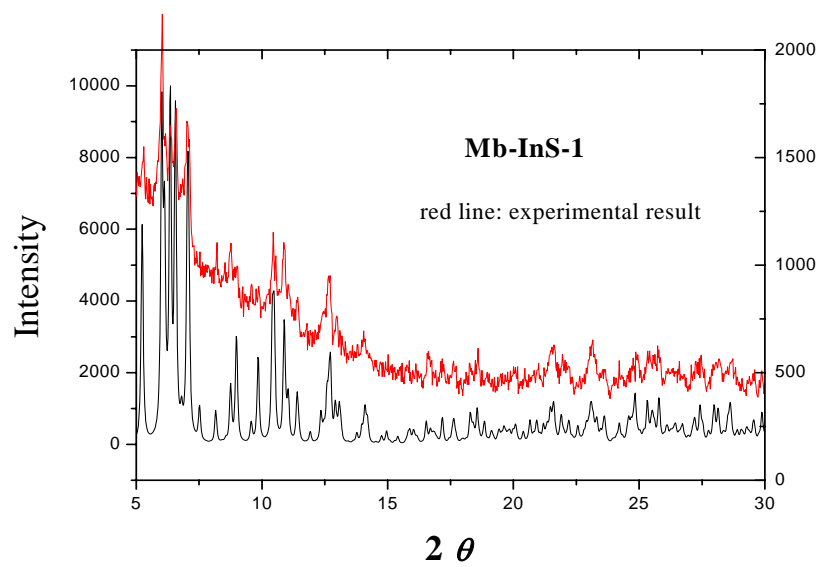


(b)

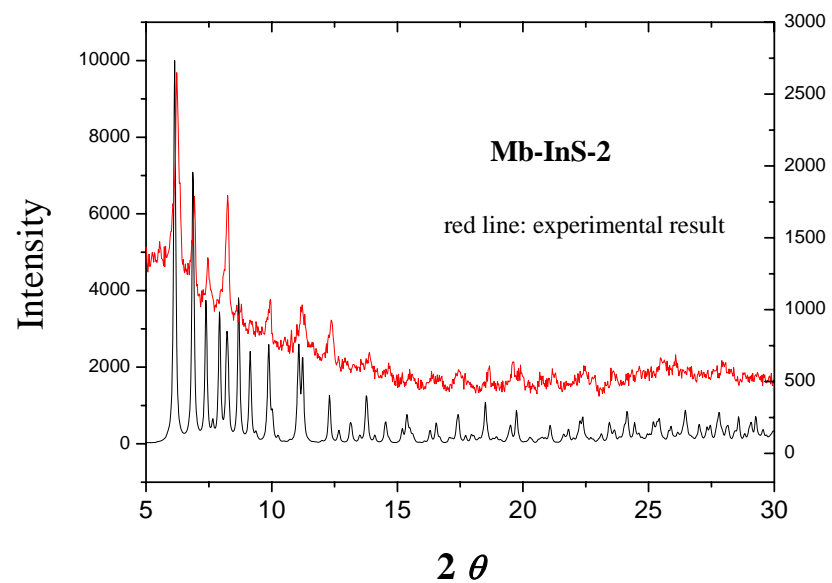


(c)

SI-Fig.-2. The IR spectra of Mb-InS-1 (a), 2 (b), and 3 (c).



(a)



(b)

**SI-Fig.-3.** PXRD patterns for the experimental and calculated results of Mb-InS-1 (a), and Mb-InS-2 (b) to assure their phase purity.

**SI-Table 1** The In-S bond lengths (Å) for complexes **Mb-InS-1~3**.

| Mb-InS-1 |     |          | Mb-InS-2 |      |          |
|----------|-----|----------|----------|------|----------|
| In1      | S2  | 2.434(5) | In1      | S2   | 2.440(4) |
| In1      | S4  | 2.452(5) | In1      | S4   | 2.445(4) |
| In1      | S3  | 2.458(5) | In1      | S3   | 2.449(4) |
| In1      | S1  | 2.481(5) | In1      | S1   | 2.485(4) |
| In2      | S5  | 2.407(5) | In2      | S2   | 2.405(4) |
| In2      | S2  | 2.411(5) | In2      | S5   | 2.410(4) |
| In2      | S7  | 2.506(5) | In2      | S6   | 2.500(4) |
| In2      | S6  | 2.518(4) | In2      | S7   | 2.517(4) |
| In3      | S3  | 2.408(5) | In3      | S8   | 2.414(4) |
| In3      | S8  | 2.419(4) | In3      | S3   | 2.416(4) |
| In3      | S6  | 2.488(5) | In3      | S9   | 2.510(4) |
| In3      | S9  | 2.495(4) | In3      | S6   | 2.514(4) |
| In4      | S4  | 2.406(5) | In4      | S4   | 2.416(4) |
| In4      | S10 | 2.415(5) | In4      | S10  | 2.419(4) |
| In4      | S7  | 2.511(5) | In4      | S9   | 2.498(4) |
| In4      | S9  | 2.515(4) | In4      | S7   | 2.515(4) |
| In5      | S13 | 2.403(8) | In5      | S13  | 2.429(4) |
| In5      | S5  | 2.436(6) | In5      | S5   | 2.431(4) |
| In5      | S12 | 2.451(5) | In5      | S12  | 2.432(5) |
| In5      | S11 | 2.479(6) | In5      | S11  | 2.475(5) |
| In6      | S12 | 2.401(5) | In6      | S14  | 2.410(5) |
| In6      | S14 | 2.407(4) | In6      | S12  | 2.415(4) |
| In6      | S15 | 2.482(5) | In6      | S15  | 2.511(4) |
| In6      | S6  | 2.507(5) | In6      | S6   | 2.515(4) |
| In7      | S13 | 2.404(6) | In7      | S16  | 2.389(4) |
| In7      | S16 | 2.425(7) | In7      | S13  | 2.410(4) |
| In7      | S7  | 2.507(5) | In7      | S15  | 2.495(4) |
| In7      | S15 | 2.519(4) | In7      | S7   | 2.507(4) |
| In8      | S8  | 2.440(5) | In8      | S19# | 2.435(4) |
| In8      | S14 | 2.441(4) | In8      | S14  | 2.450(5) |
| In8      | S18 | 2.442(5) | In8      | S17  | 2.459(4) |
| In8      | S17 | 2.488(4) | In8      | S8   | 2.465(4) |
| In9      | S19 | 2.401(5) | In9      | S18  | 2.413(4) |
| In9      | S18 | 2.419(4) | In9      | S17  | 2.419(4) |
| In9      | S15 | 2.497(5) | In9      | S9   | 2.497(4) |
| In9      | S9  | 2.508(4) | In9      | S15  | 2.515(4) |
| In10     | S10 | 2.437(5) | In10     | S18  | 2.449(4) |
| In10     | S19 | 2.438(5) | In10     | S19  | 2.452(4) |
| In10     | S16 | 2.446(7) | In10     | S16  | 2.455(4) |
| In10     | S20 | 2.474(7) | In10     | S10  | 2.465(4) |

#: 1/2-x, 1/2-y, 1/2-z

| Mb-InS-3 |       |          |
|----------|-------|----------|
| In1      | S2    | 2.451(6) |
| In1      | S3    | 2.459(6) |
| In1      | S1    | 2.465(6) |
| In1      | S4    | 2.483(6) |
| In2      | S5    | 2.419(6) |
| In2      | S2    | 2.421(6) |
| In2      | S7    | 2.500(5) |
| In2      | S6    | 2.506(5) |
| In3      | S3    | 2.422(6) |
| In3      | S8    | 2.432(6) |
| In3      | S6    | 2.494(6) |
| In3      | S9    | 2.511(5) |
| In4      | S10   | 2.413(6) |
| In4      | S4    | 2.419(5) |
| In4      | S9    | 2.498(5) |
| In4      | S7    | 2.517(5) |
| In5      | S35## | 2.424(6) |
| In5      | S11   | 2.442(5) |
| In5      | S5    | 2.454(6) |
| In5      | S12   | 2.476(5) |
| In6      | S11   | 2.385(5) |
| In6      | S13   | 2.406(6) |
| In6      | S14   | 2.508(6) |
| In6      | S6    | 2.518(6) |
| In7      | S15   | 2.415(5) |
| In7      | S12   | 2.424(5) |
| In7      | S7    | 2.501(5) |
| In7      | S14   | 2.508(5) |
| In8      | S16   | 2.421(4) |
| In8      | S13   | 2.444(6) |
| In8      | S17   | 2.450(6) |
| In8      | S8    | 2.460(6) |
| In9      | S18   | 2.393(5) |
| In9      | S17   | 2.409(5) |
| In9      | S14   | 2.487(5) |
| In9      | S9    | 2.502(5) |
| In10     | S19   | 2.441(5) |
| In10     | S15   | 2.448(6) |
| In10     | S18   | 2.459(5) |
| In10     | S10   | 2.460(6) |

| Mb-InS-3 |     |          |
|----------|-----|----------|
| In11     | S21 | 2.438(5) |
| In11     | S22 | 2.441(6) |
| In11     | S23 | 2.456(6) |
| In11     | S20 | 2.463(6) |
| In12     | S24 | 2.411(5) |
| In12     | S21 | 2.415(5) |
| In12     | S26 | 2.493(6) |
| In12     | S25 | 2.529(6) |
| In13     | S27 | 2.398(5) |
| In13     | S22 | 2.410(5) |
| In13     | S28 | 2.499(5) |
| In13     | S25 | 2.503(5) |
| In14     | S29 | 2.394(5) |
| In14     | S23 | 2.424(5) |
| In14     | S26 | 2.513(5) |
| In14     | S28 | 2.521(5) |
| In15     | S19 | 2.432(5) |
| In15     | S30 | 2.435(5) |
| In15     | S24 | 2.454(5) |
| In15     | S31 | 2.470(5) |
| In16     | S32 | 2.395(5) |
| In16     | S30 | 2.406(5) |
| In16     | S25 | 2.499(5) |
| In16     | S33 | 2.510(5) |
| In17     | S34 | 2.388(5) |
| In17     | S31 | 2.402(5) |
| In17     | S26 | 2.472(5) |
| In17     | S33 | 2.506(5) |
| In18     | S35 | 2.431(5) |
| In18     | S32 | 2.461(5) |
| In18     | S36 | 2.479(6) |
| In18     | S27 | 2.489(5) |
| In19     | S37 | 2.370(6) |
| In19     | S36 | 2.396(5) |
| In19     | S33 | 2.512(5) |
| In19     | S28 | 2.525(5) |
| In20     | S38 | 2.419(4) |
| In20     | S37 | 2.453(5) |
| In20     | S34 | 2.462(5) |
| In20     | S29 | 2.481(5) |

##: x, 1+y, z.