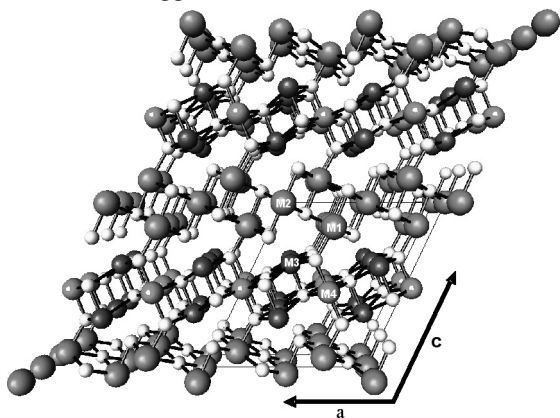


Synthesis and Characterization of Quaternary Chalcogenide $\text{In}_1\text{Sn}_2\text{Bi}_3\text{Se}_8$. Ming-Fang Wang, Chi-Shen Lee^{1*}, Chia-Jyi Liub², ¹Dept. of Applied Chemistry and Inst. of Molecular Science, National Chiao Tung Univ., 1001 Ta-Hsueh Rd., Hsinchu 30010, Taiwan, ²Dept. of Physic, National Changhua Univ. of Education, 1 Jin-De Road, Changhua, Taiwan 500, Republic of China.

A new quaternary compound $\text{In}_2\text{Sn}_4\text{Bi}_6\text{Se}_{16}$ was synthesized by direct combinations of the In:Sn:Bi:Se = 1:2:3:8 at 1023 K. The compound crystallized in the monoclinic space group $C2/m$ with $a = 13.557(3) \text{ \AA}$, $b = 4.1299(8) \text{ \AA}$, $c = 15.252(3) \text{ \AA}$, $\beta = 115.73(3)^\circ$, $V = 769.3(3) \text{ \AA}^3$, $Z = 1$, and $R_1/wR_2/\text{GOF} = 0.0213/0.052/1.089$. The structure of $\text{In}_1\text{Sn}_2\text{Bi}_3\text{Se}_8$ features three-dimensional framework consisting of rectangular NaCl-type infinite rod unit running parallel to the a -axis, which are stitched together by Bi-Se. Electronic structure calculation based on the model $\text{In}_2\text{Sn}_4\text{Bi}_6\text{Se}_{16}$ suggests that the material is a narrow band gap semiconductor. Thermopower of $\text{In}_1\text{Sn}_2\text{Bi}_3\text{Se}_8$ is -270



$(20) \mu\text{V/K}$ over temperature range between 300 and 700 K. Electrical conductivity and thermal conductivity of $\text{In}_1\text{Sn}_2\text{Bi}_3\text{Se}_8$ at room temperature are $1645(7) \text{ Sm}^{-1}$ and 0.36 W/mK , respectively, which indicating the Figure of Merit (ZT) at room temperature close to 0.1.

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Perspective view of the structures of $\text{InSn}_2\text{Bi}_3\text{Se}_8$ along the b -axis.