Supporting information

The Zintl phases $A In_2As_2$ (A = Ca, Sr, Ba): New topological insulators and thermoelectric material candidates

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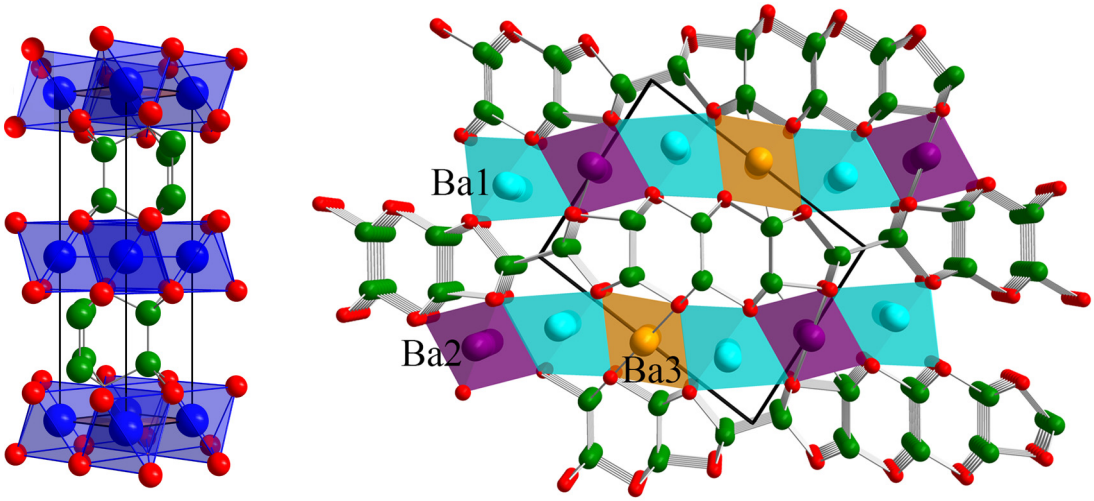

Figure S1. The structures of $CaIn_2As_2$ ($P6_3/mmc$) and $BaIn_2As_2$ ($P2/m$) showing the coordination polyhedra of the cations and their packing arrangement. The three unique crystallographic positions for the Ba atoms in the $BaIn_2As_2$ structure are differentiated as turquoise, purple and, marigold spheres, respectively.

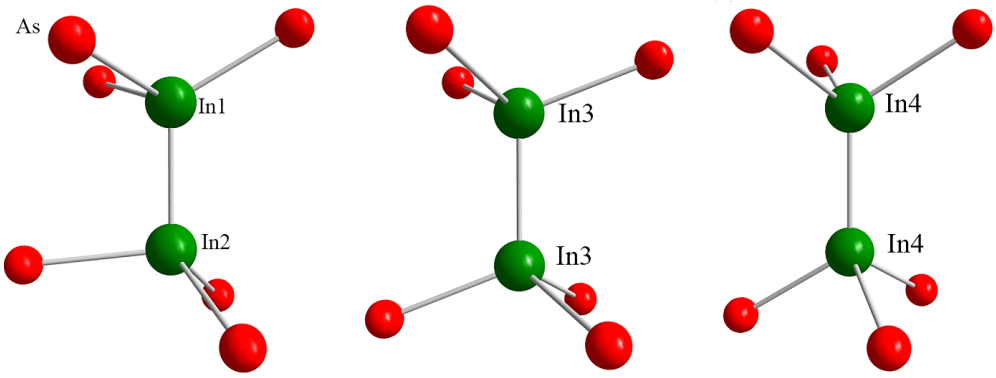

Figure S2. The three different ethane-like units that makes up the $[In_2As_2]^{2-}$ slabs in the $BaIn_2As_2$ structure.

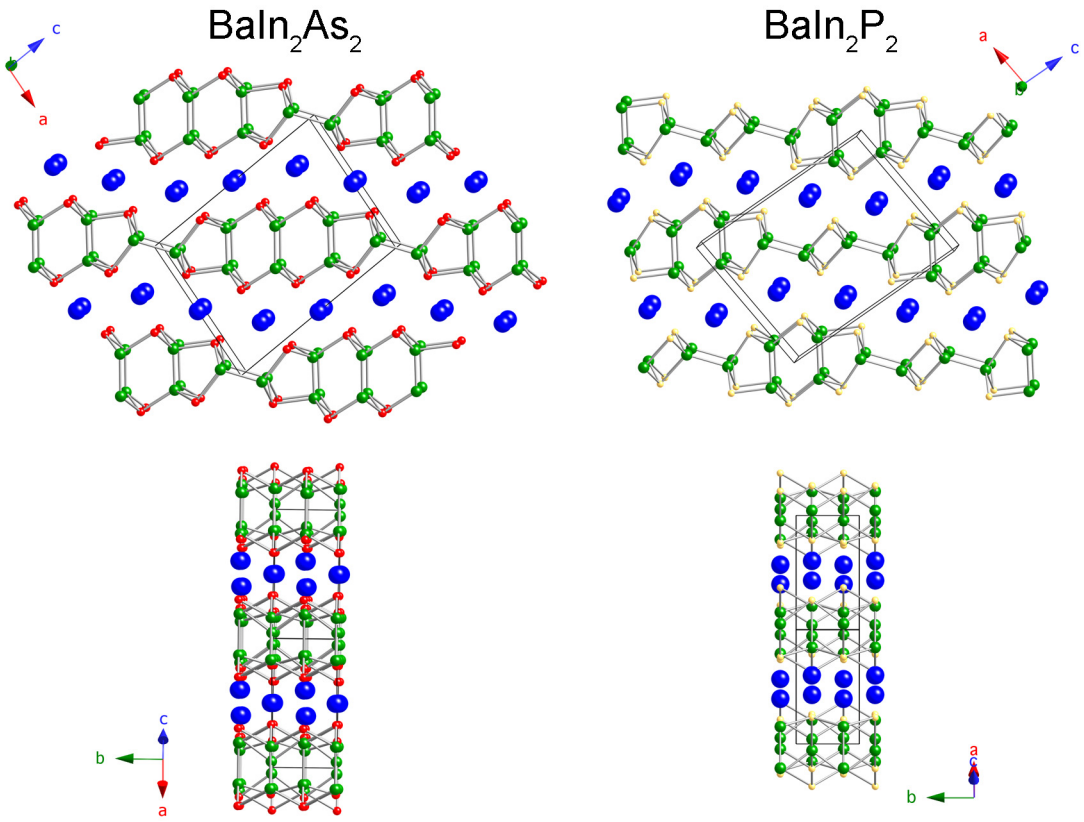

Figure S3. The structures of $BaIn_2As_2$ ($P2/m$) and $BaIn_2P_2$ ($P2_1/m$).

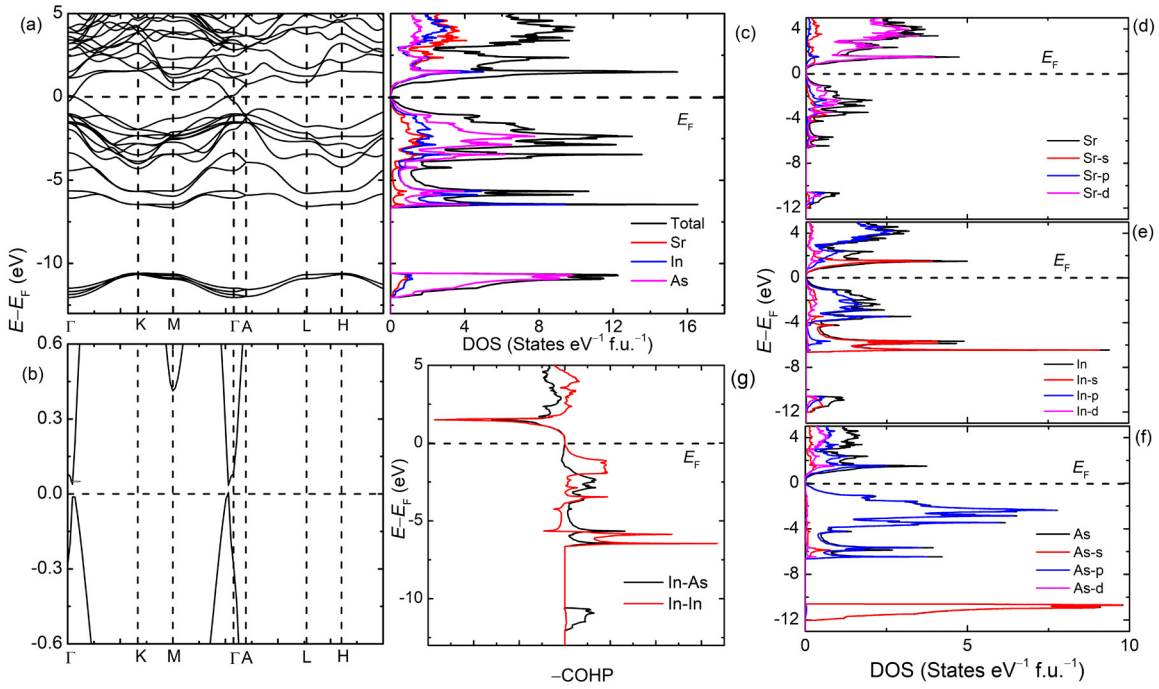

Figure S4. (a): Calculated bulk electronic band structure of $SrIn_2As_2$ along high symmetry directions. The Fermi level is taken as $E-E_F = 0$ and represented with dashed lines. (b): A zoomed-in view of the band structure for small energy window close to the Fermi level which reveals a small direct band gap opening along the Γ point. (c): Total density of states of $CaIn_2As_2$ together with the partial density of states for Sr, In and As. (d) to (f) Orbital resolved partial DOS curves. (g): COHP curves evaluated for the average In−In and As−As bonds

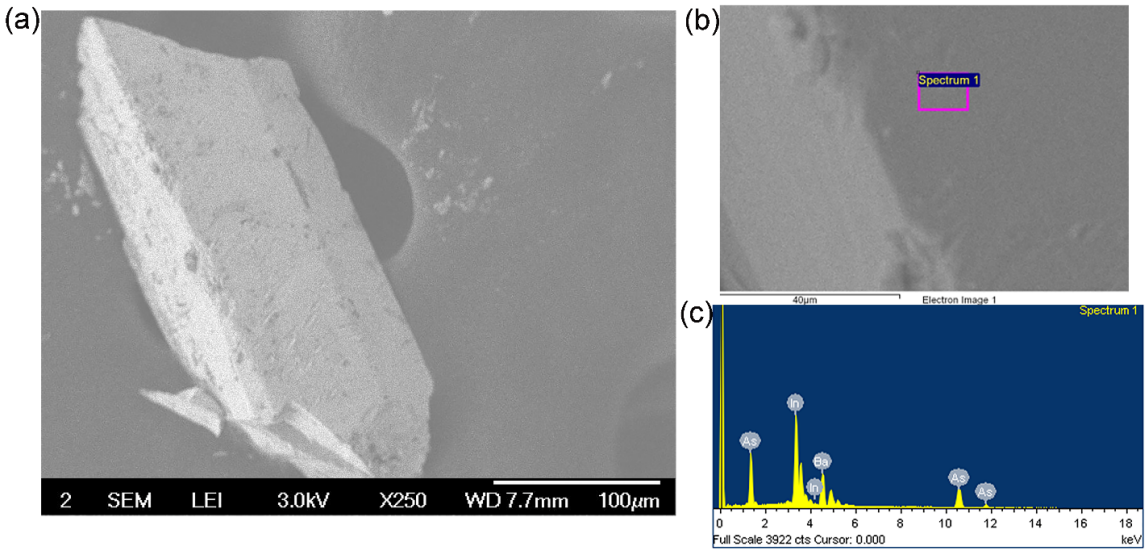

Figure S5. (a) SEM image of a $BaIn_2As_2$ crystal. (b) SEM image under higher magnification of the same $BaIn_2As_2$ crystal; the enclosed area is where the elemental composition was probed. (c) Histogram from the EDS analysis for $BaIn_2As_2$. The abscissa shows the energy in units keV and the *y*-axis shows the intensities (counts). Elemental analysis confirms only three elements in the chemical makeup of the studied specimen, and their stoichiometric ratio is in agreement with the chemical formula $BaIn_2As_2$.