

## Supplementary information

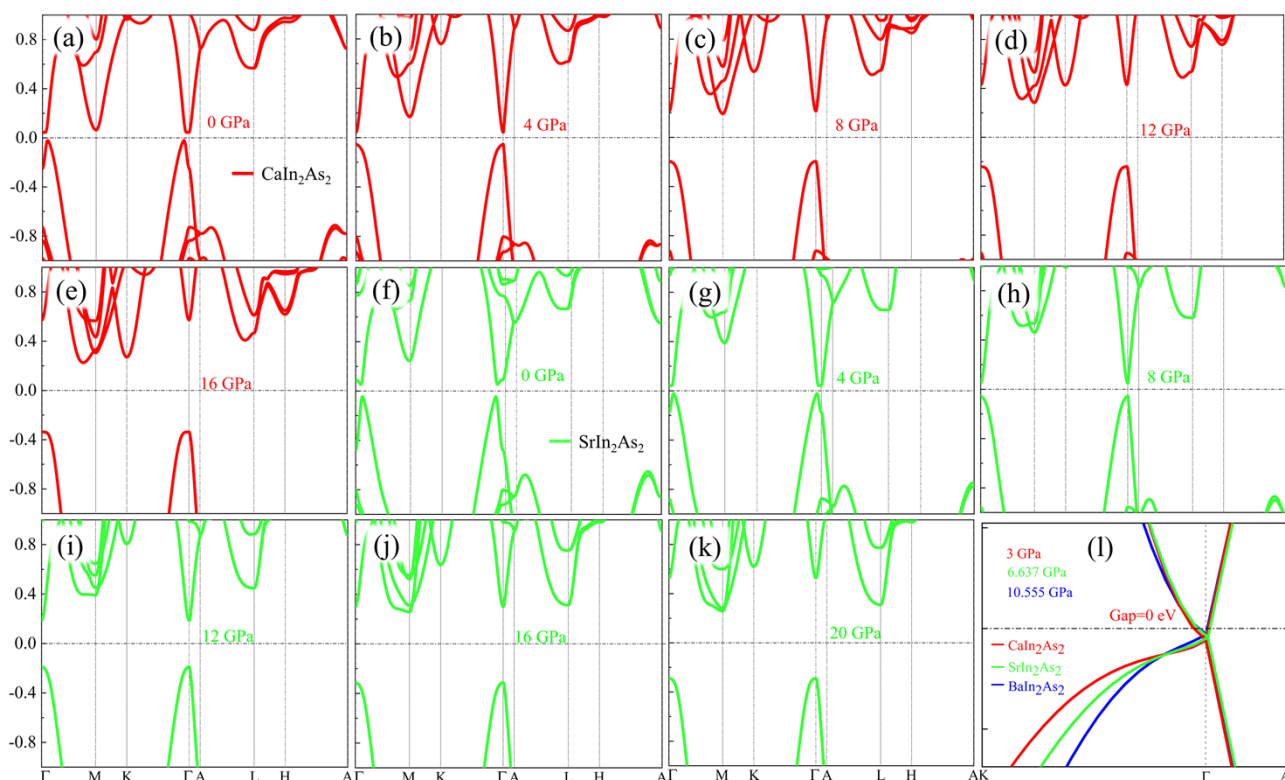
### The Zintl phases compound $\text{AEIn}_2\text{As}_2$ (AE=Ca, Sr, Ba): topological phase transition under pressure

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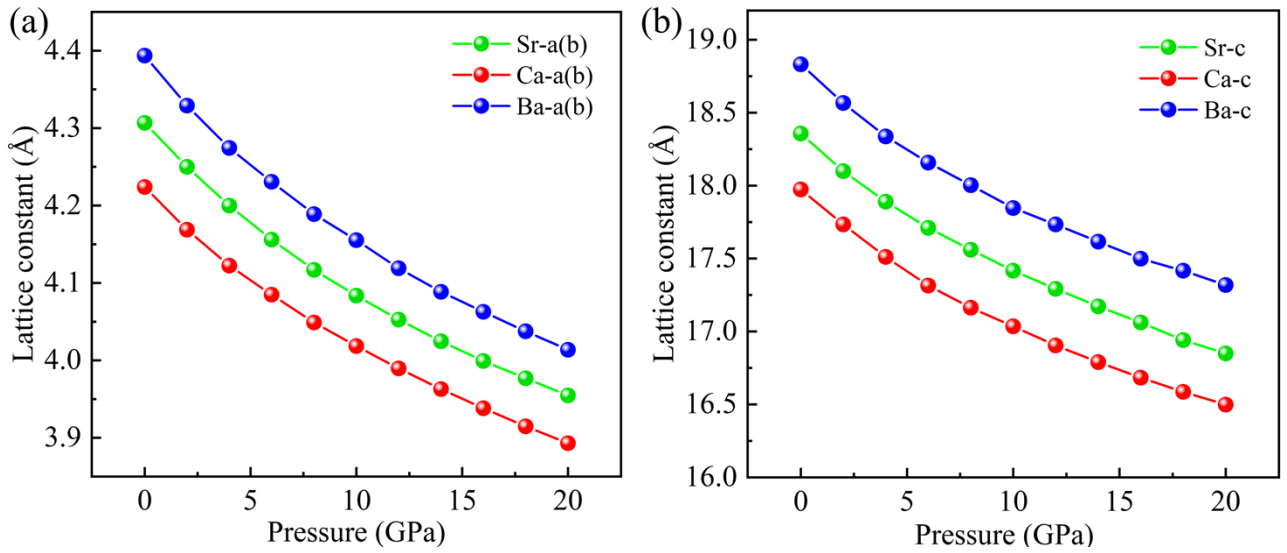
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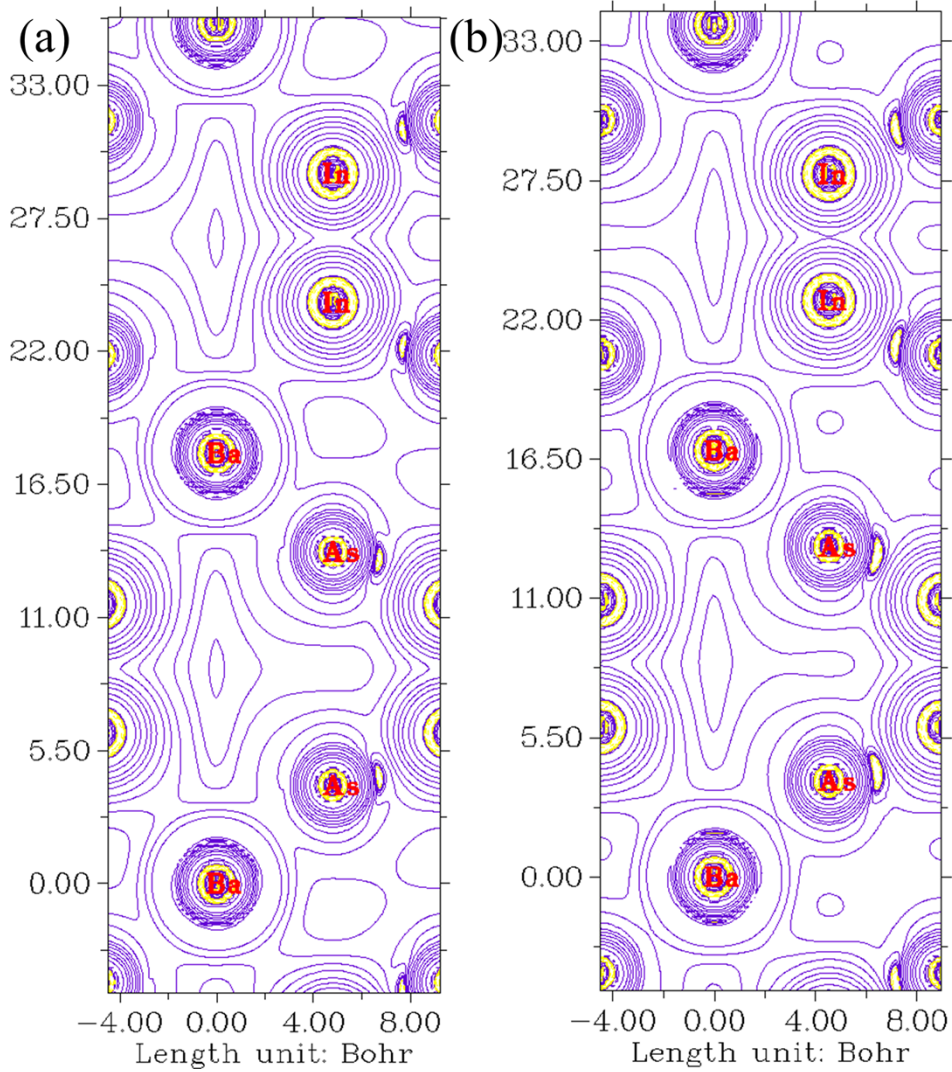
(\*E-mail: [jmzhang@fjnu.edu.cn](mailto:jmzhang@fjnu.edu.cn))



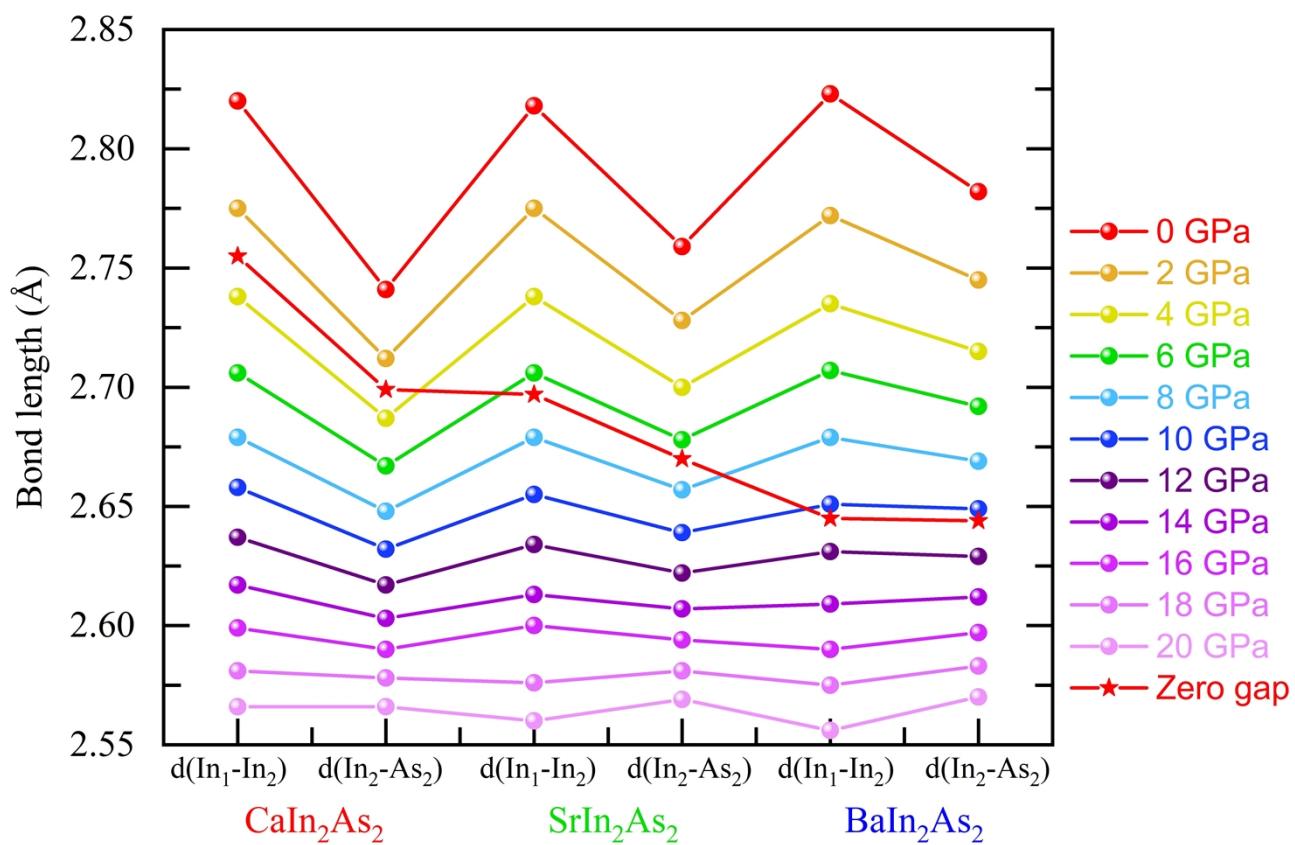
**Fig. S1** Band structures of (a-e)  $\text{CaIn}_2\text{As}_2$  and (f-k)  $\text{SrIn}_2\text{As}_2$  under pressure. (l) Band structures of hydrostatic pressure-induced  $\text{AEIn}_2\text{As}_2$  with zero band gap.



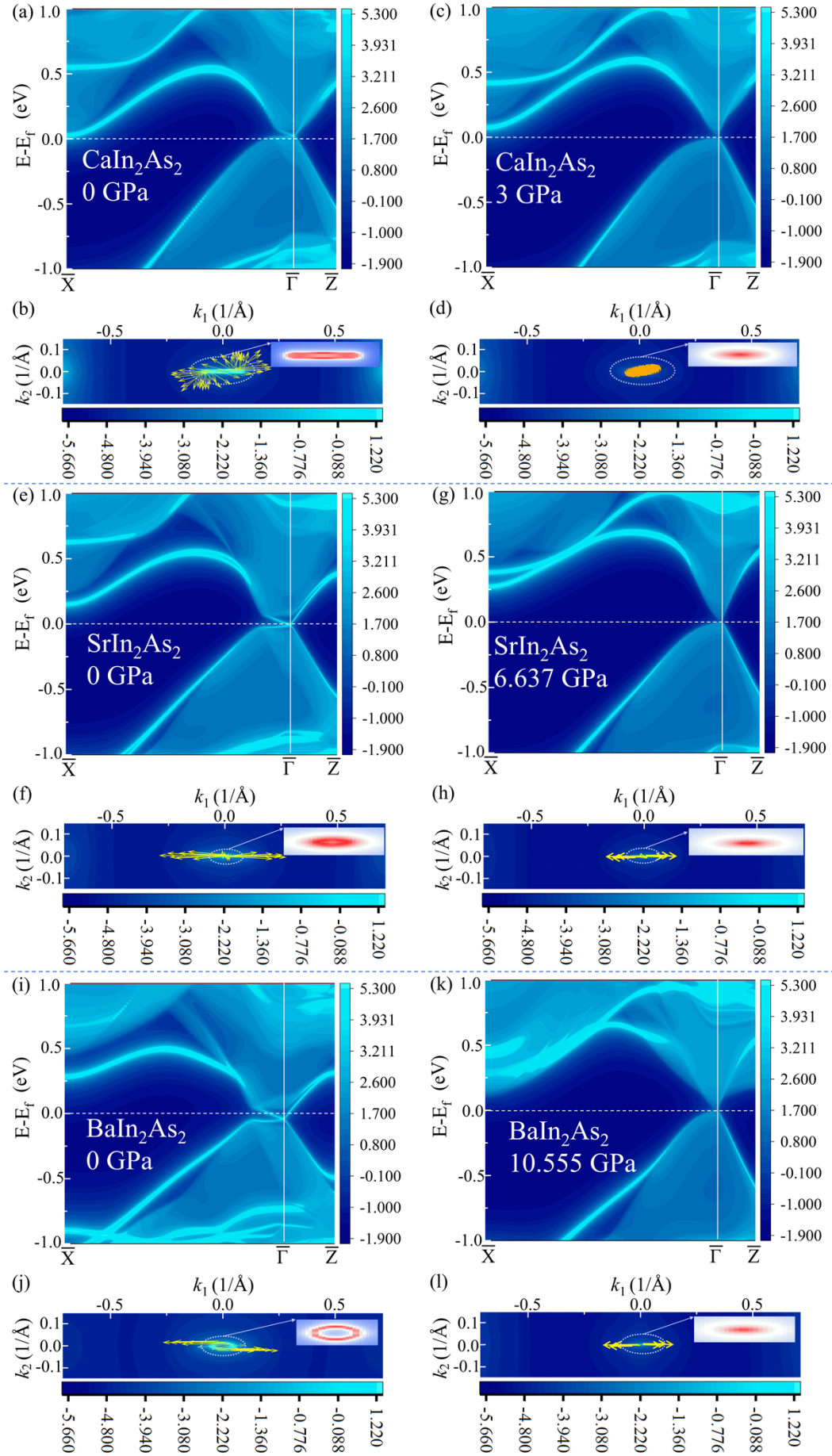
**Fig. S2** Evolutionary regular curve of  $\text{AEIn}_2\text{As}_2$  of the lattice constants (a)  $a$  or  $b$  and (b)  $c$  direction.



**Fig. S3**  $d^2\rho$  isolines of  $\text{BaIn}_2\text{As}_2$  under (a) 0 GPa (b) 10.555 GPa in the (100) plane at the equilibrium geometry. Yellow lines correspond to negative isovalues of charge accumulation, while purple lines correspond to positive isovalues of charge depletion.



**Fig. S4** Bond length evolution of In<sub>1</sub>-In<sub>2</sub> and In<sub>2</sub>-As<sub>2</sub> chemical bonds in the AEIn<sub>2</sub>As<sub>2</sub> system under different pressures.



**Fig. S5** Surface states of the (010) surface and corresponding Fermi Surfaces (FS) contain spin

texture at the Fermi level for the three  $A\text{EInIn}_2\text{As}_2$  systems under atmospheric pressure and induced zero band gap pressure. The surface state results for  $\text{CaIn}_2\text{As}_2$ ,  $\text{SrIn}_2\text{As}_2$ , and  $\text{BaIn}_2\text{As}_2$  are separated by blue dashed lines, respectively.