

*Supplementary Information for*

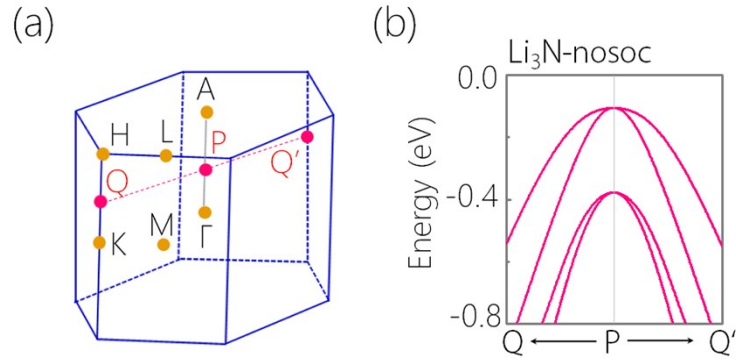
**Electronic structure, doping effect and topological signature in  
realistic intermetallics  $\text{Li}_{3-x}\text{Na}_x\text{M}$  ( $x=3, 2, 1, 0$ ;  $\text{M}=\text{N}, \text{P}, \text{As}, \text{Sb}, \text{Bi}$ )**

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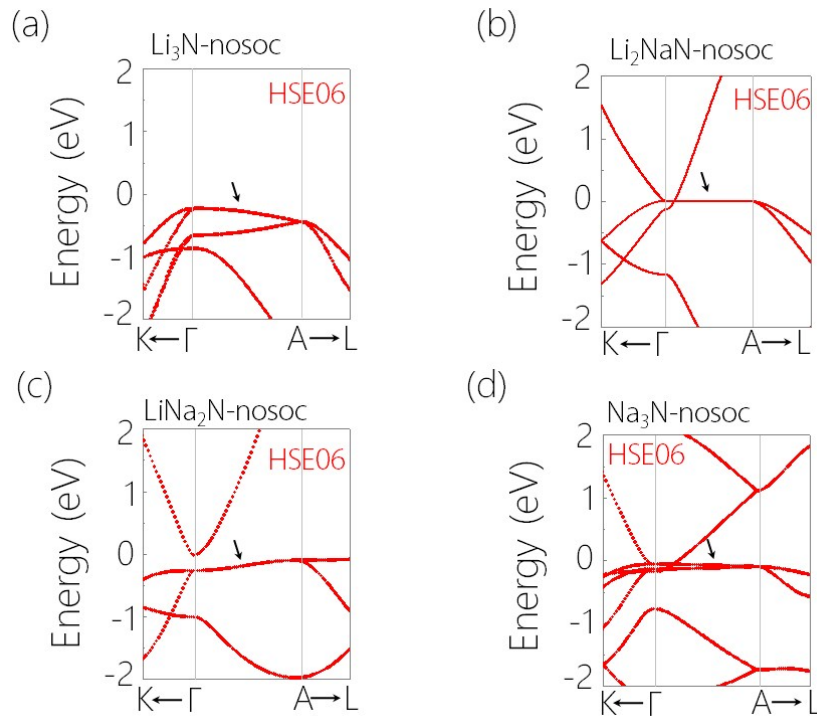
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## I. Band structure in the $k$ -path perpendicular to $\Gamma$ -A

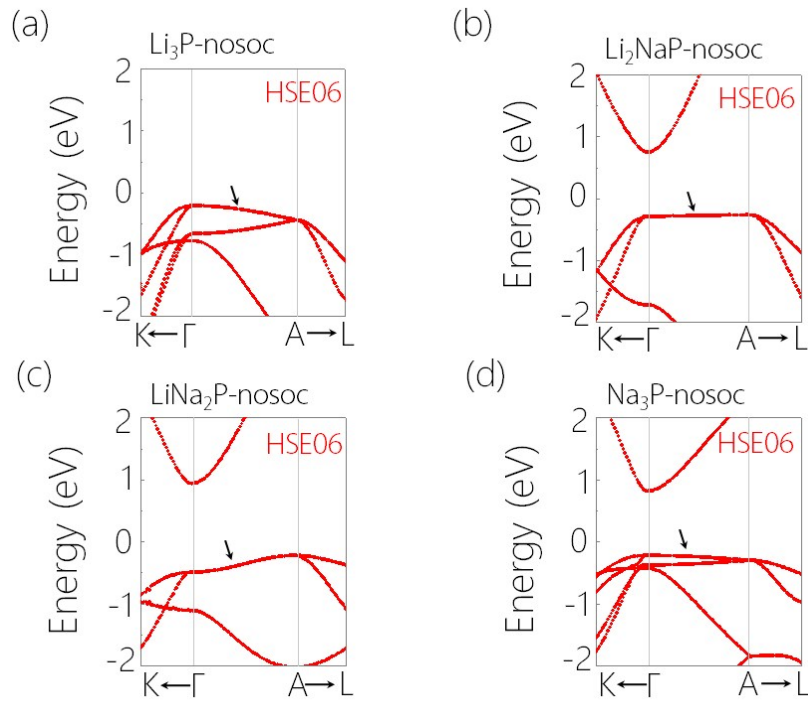


**Figure S1.** (a) The bulk Brillouin zone.  $P$  point locates on  $\Gamma$ - $A$  high-symmetry line.  $Q$  and  $Q'$  are two points in the (100) direction. (b) Enlarged view of band structure of Li<sub>3</sub>N along the  $Q$ - $P$ - $Q'$  path. It shows the band dispersion in the (100) direction around the NL.

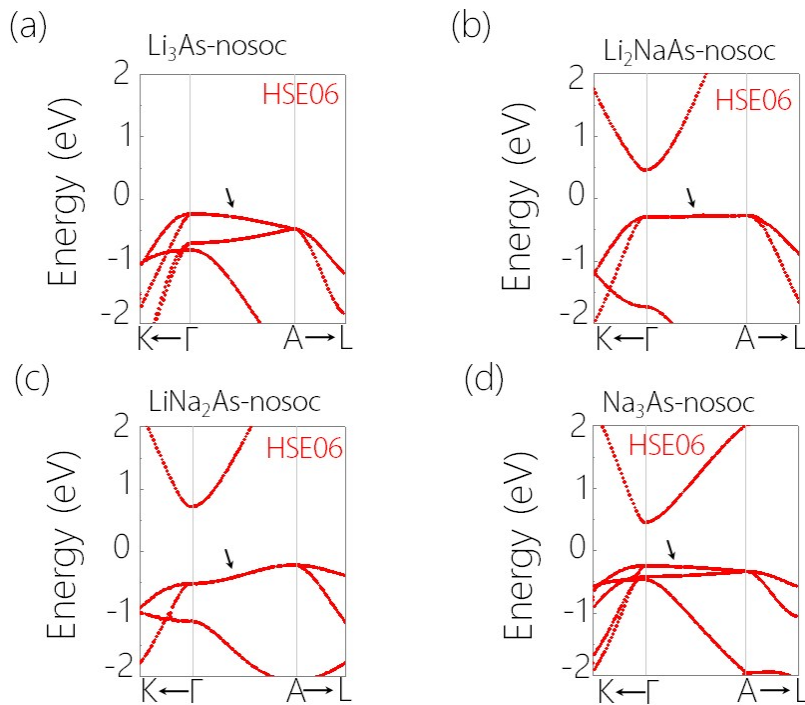
## II. Band structures under HSE06 potential



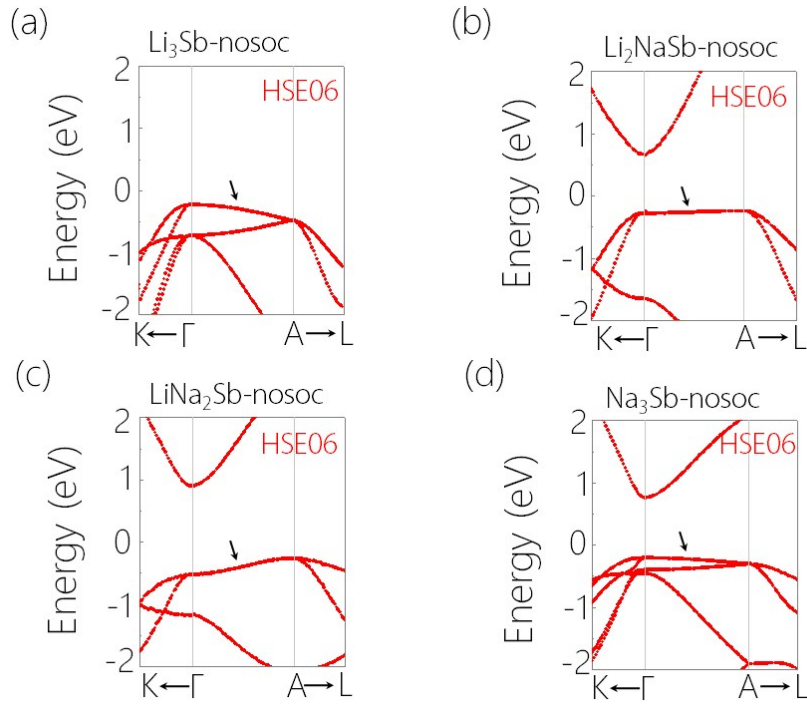
**Figure S2.** Electronic band structures of (a) Li<sub>3</sub>N, (b) Li<sub>2</sub>NaN, (c) LiNa<sub>2</sub>N and (d) Na<sub>3</sub>N by HSE06 hybrid functional. The arrows point out the NLs.



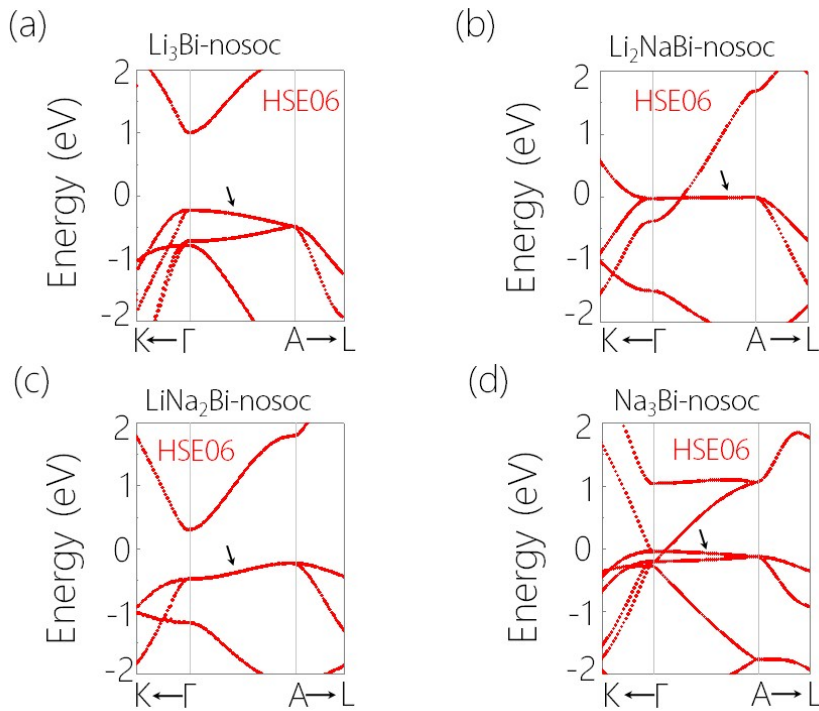
**Figure S3.** Electronic band structures of (a)  $\text{Li}_3\text{P}$ , (b)  $\text{Li}_2\text{NaP}$ , (c)  $\text{LiNa}_2\text{P}$  and (d)  $\text{Na}_3\text{P}$  by HSE06 hybrid functional. The arrows point out the NLs.



**Figure S4.** Electronic band structures of (a)  $\text{Li}_3\text{As}$ , (b)  $\text{Li}_2\text{NaAs}$ , (c)  $\text{LiNa}_2\text{As}$  and (d)  $\text{Na}_3\text{As}$  by HSE06 hybrid functional. The arrows point out the NLs.



**Figure S5.** Electronic band structures of (a)  $\text{Li}_3\text{Sb}$ , (b)  $\text{Li}_2\text{NaSb}$ , (c)  $\text{LiNa}_2\text{Sb}$  and (d)  $\text{Na}_3\text{Sb}$  by HSE06 hybrid functional. The arrows point out the NLs.



**Figure S6.** Electronic band structures of (a)  $\text{Li}_3\text{Bi}$ , (b)  $\text{Li}_2\text{NaBi}$ , (c)  $\text{LiNa}_2\text{Bi}$  and (d)  $\text{Na}_3\text{Bi}$  by HSE06 hybrid functional. The arrows point out the NLs.