Supplementary material

Electric field and strain tunable band gap and band alignments of $MoSi_2N_4$/MSe (M = In, Ga) van der Waals heterostructures

Jin Quan Ng, Qingyun Wu, L. K. Ang[1],* and Yee Sin Ang*
[1]*Science, Mathematics and Technology, Singapore University of Technology and Design (SUTD), 8 Somapah Road, 487372, Singapore*

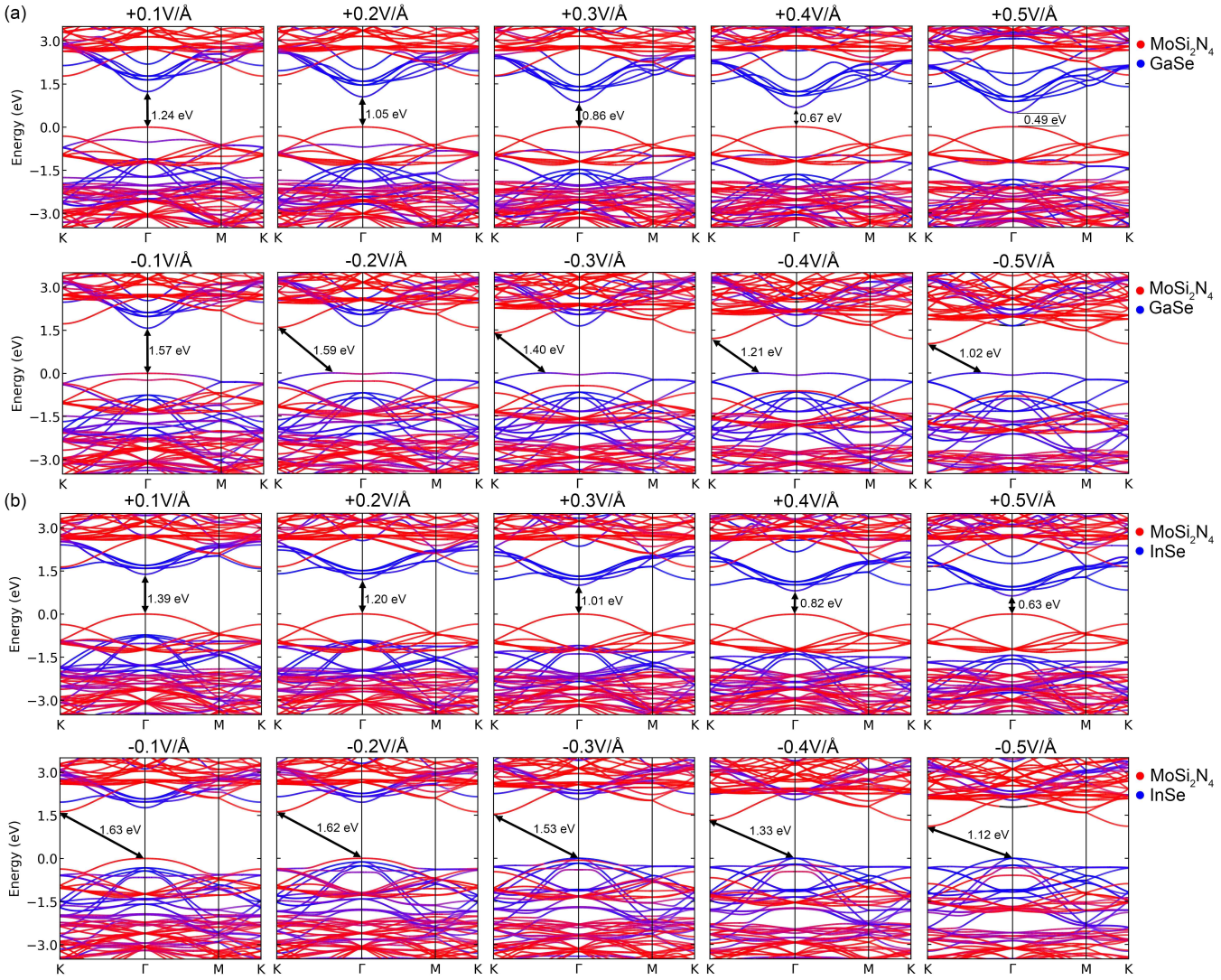

Fig. S 1. Band structures of (a) $MoSi_2N_4$/GaSe (b) $MoSi_2N_4$/InSe under external electric field. Vacuum states exist at higher external electric field, but have low electron counts and hence negligible effect on band gap for included range.

* Authors to whom correspondence should be addressed: ricky_ang@sutd.edu.sg and yeesin_ang@sutd.edu.sg

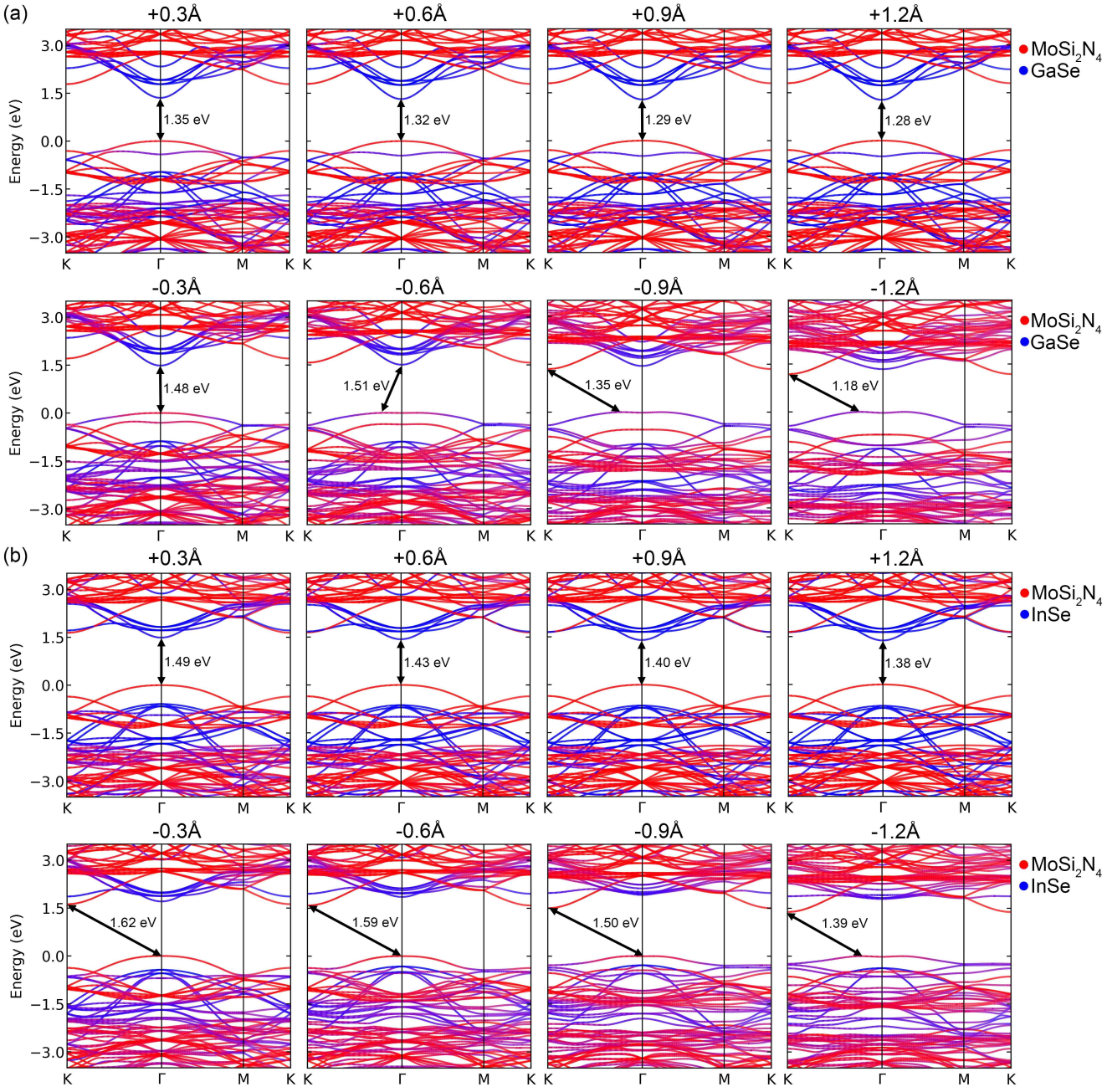

Fig. S 2. Band structures of (a) $MoSi_2N_4$/GaSe (b) $MoSi_2N_4$/InSe under vertical strain. Negative vertical strain is compressive.

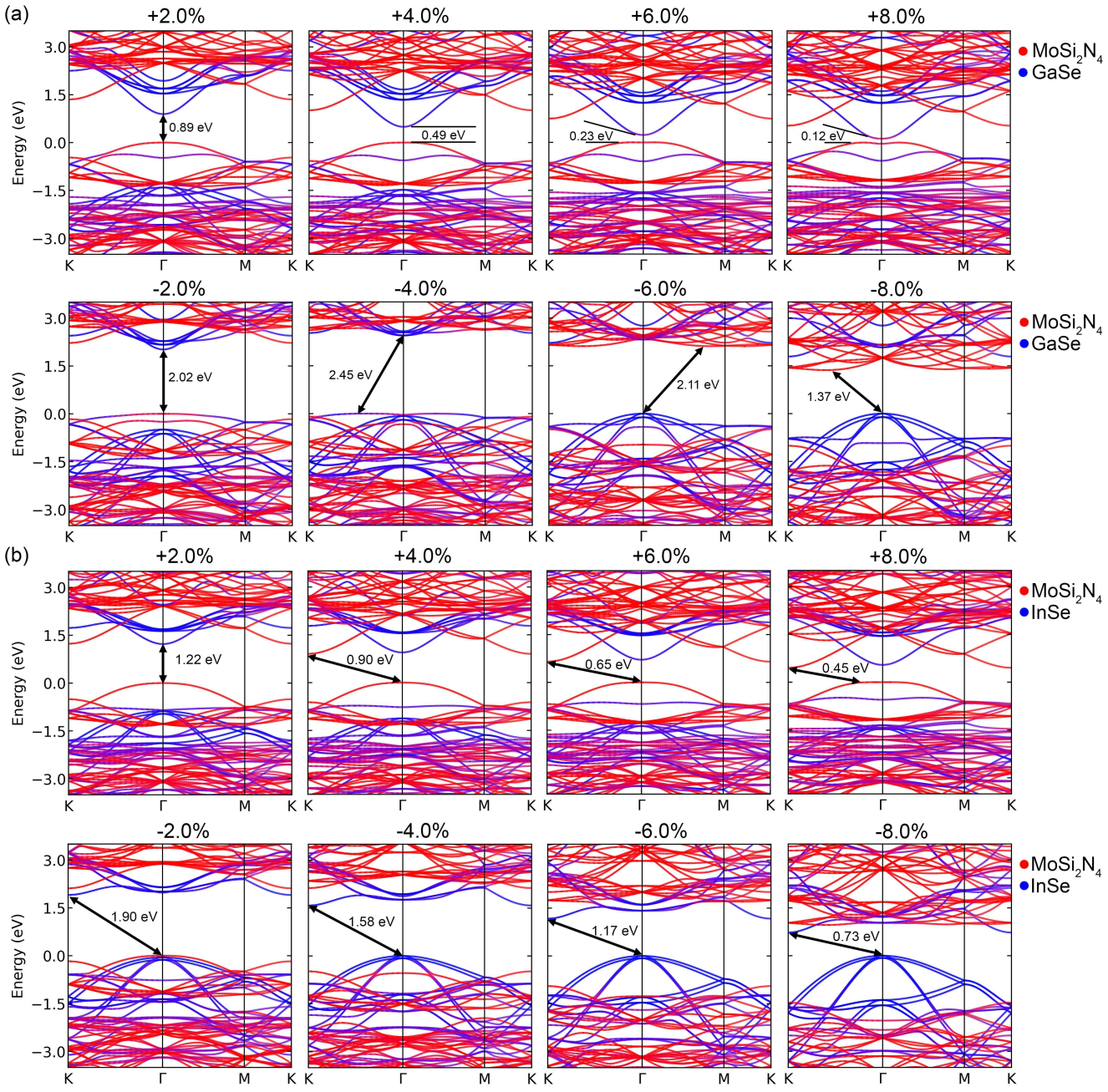

Fig. S 3. Band structures of (a) $MoSi_2N_4$/GaSe (b) $MoSi_2N_4$/InSe under biaxial strain. Negative biaxial strain is compressive.