Supporting Information for

"Electronic and photochemical properties of hybrid binary silicon and germanium derived Janus monolayers"

*Xiuyuan Li*¹, *Kaining Zhang*¹, *Xin Zeng*¹, *Nan Li*^{*1} and *Jichang Wang*^{*2}

- State Key Laboratory of Explosion Science and Technology, School of Mechatronical Engineering, Beijing Institute of Technology, Beijing 100081, P. R. China.
- 2. Department of Chemistry and Biochemistry, University of Windsor, Windsor,

Ontario N9B 3P4, Canada

*Corresponding author:

Nan Li	Jichang Wang
E-mail: leen04@bit.edu.cn	E-mail:jwang@uwindsor.ca
Phone: +86-010-68914863	Phone:1-519-253-3000 ext. 3540



Fig. S1 The side view of optimized lattice structures of (a) Si₂NP, (b)Si₂NAs, (c) Si₂PAs, (d) Ge₂NP (e) Ge₂NAs and (f) Ge₂PAs.



Fig. S2 Band structures of ML (a) SiN, (b)SiP, (c) SiAs, (d) GeN,(e) GeP and(f) GeAs calculated at the theory level of PBE. The horizontal dash line located at 0 eV represents the Fermi level.



Fig. S3 Top view of ML Si₂NP, d is the distance of neighboring Si atoms.



Fig. S4 Band structures of ML (a)Si₂NAs, (b) Si₂PAs, (c) Ge₂NP and (d) Ge₂PAs calculated at the theory level of PBE+SOC. The horizontal dash line located at 0 eV represents the Fermi level.



Fig. S5 Partial charge densities of GeP: (a) CBM, (b) VBM and GeAs:(c) CBM, (d) VBM with an isosurface of 0.002 eÅ⁻³.