Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for

"High Stability and Visible-Light Photocatalysis in Novel Two-Dimensional Monolayer Silicon and Germanium Mononitride Semiconductors: First-Principles Study"

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Table S1 Bond lengths of MLs GeN and GeP.

	d_{GeGe1}/Å	d_{GeGe2}/Å
GeN	2.488	2.482
GeP	2.494	2.499

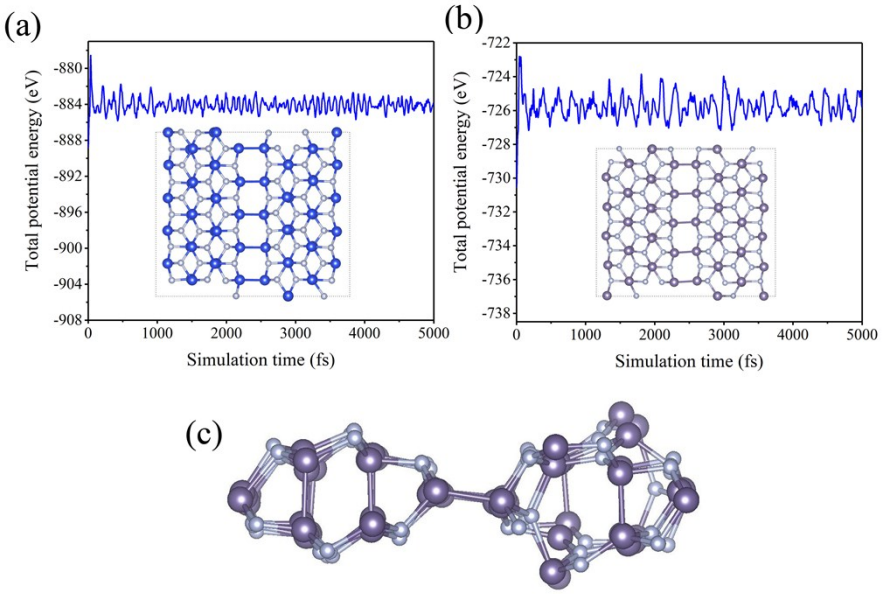

Fig. S1 The evolution of total energies of MLs (a) SiN and (b) GeN with T = 300 K. The insets show snapshots of supercells at the end of 5 ps. (c) The lattice structure of ML GeN with T = 1000 K at the end of 5 ps.

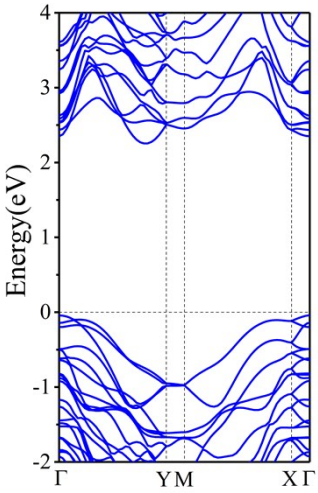

Fig.S2 Band structure of ML GeP at HSE06 level of theory. The horizontal dash line located at 0 eV represents the Fermi level.

Supplementary Note 1: Detailed discussion of different band gaps

Here we take ML GeN and GeP as an example to discuss the mechanism. By comparing the band structures of ML GeN (Fig. 3b) and GeP (Fig. S2), we observe that their VBMs lie near the Fermi level, while the CBM of GeN is lower than that of GeP, resulting in a smaller band gap of GeN. The in-depth partial density of states (PDOS) (Fig. 3d) show that the CBM of ML GeN is mostly made of the 4*s* orbitals of Ge at Γ point and these orbitals undergo strong interactions. At Γ point, these interactions are bonding along the GeGe1 and GeGe2 bonds direction (defined in Fig. 1), so that when the GeGe1 and GeGe2 bond lengths decrease/increase the energy of CBM is decrease/increase. The ML GeP can be obtained through replacing the N atoms in GeN by P atoms. The GeGe1 and GeGe2 bonds in GeP are longer than those in GeN due to the larger atomic radius of P compared to N atom (see Table S1), which decrease the interaction between the 4*s* orbitals of Ge and lead to the increase of the energy of CBM. Therefore, the ML GeP has a larger band gap than the ML GeN.