Supporting Materials

Janus MoAZ₃H (A=Ge, Si; Z=N, P, As) monolayers: a new type of semiconductors exhibit excellent photovoltaic and catalytic performances

Xiaolin Cai¹*, Guoxing Chen¹, Rui Li¹, Weiyang Yu¹, Xuefeng Yang¹, Yu Jia²,³*

¹School of Physics and Electronic Information Engineering, Henan Polytechnic University, Jiaozuo 454000, China
²Key Laboratory for Special Functional Materials of Ministry of Education, Collaborative Innovation Center of Nano Functional Materials and Applications, School of Material Science and Engineering, Henan University, Kaifeng 475004, China
³International Laboratory for Quantum Functional Materials of Henan, and School of Physics and Microelectronics, Zhengzhou University, Zhengzhou 450001, China

Fig S1. AIMD simulation of MoAZ₃H ML material, in which the green curve is the evolution of the energy per atom over time, and the top and bottom insets are the initial and final structures, respectively.
Fig S2. Polar diagrams of Young modulus, shear modulus and Poisson ratio of MoAZ$_3$H ML.
**Fig S3.** Band structure diagram of MoAZ$_3$H ML calculated by PBE+SOC (red lines) and HSE+SOC (blue lines) functionals, with Fermi energy level set to 0.

**Fig S4.** (a) Top view of the rectangular unit cell and (b) the corresponding high symmetry path in the Brillouin zone for the MoAZ$_3$H ML.
**Fig S5.** In-plane stiffness and deformation potential of the MoSiN<sub>H</sub> ML obtained from the PBE+SOC scheme.

**Fig S6.** In-plane stiffness and deformation potential of the MoSiP<sub>H</sub> ML obtained from the PBE+SOC scheme.
Fig S7. In-plane stiffness and deformation potential of the MoSiAs$_2$H ML obtained from the PBE+SOC scheme.

Fig S8. In-plane stiffness and deformation potential of the MoGeN$_3$H ML obtained from the PBE+SOC scheme.
Fig S9. In-plane stiffness and deformation potential of the MoGeP$_3$H ML obtained from the PBE+SOC scheme.

Fig S10. In-plane stiffness and deformation potential of the MoGeAs$_3$H ML obtained from the PBE+SOC scheme.