Supporting Materials

Novel vallytronic and piezoelectric properties coexisting in Janus MoAZ$_3$H (A=Ge, Si; Z=N, P, As) monolayer

Xiaolin Cai[a*], Guoxing Chen[a], Rui Li[a], Zhixiang Pan[a], Yu Jia[b, c*]

[a]*School of Physics and Electronic Information Engineering, Henan Polytechnic University, Jiaozuo 454000, China*

[b]*Key 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*

[c]*International Laboratory for Quantum Functional Materials of Henan, and School of Physics and Microelectronics, Zhengzhou University, Zhengzhou 450001, China*
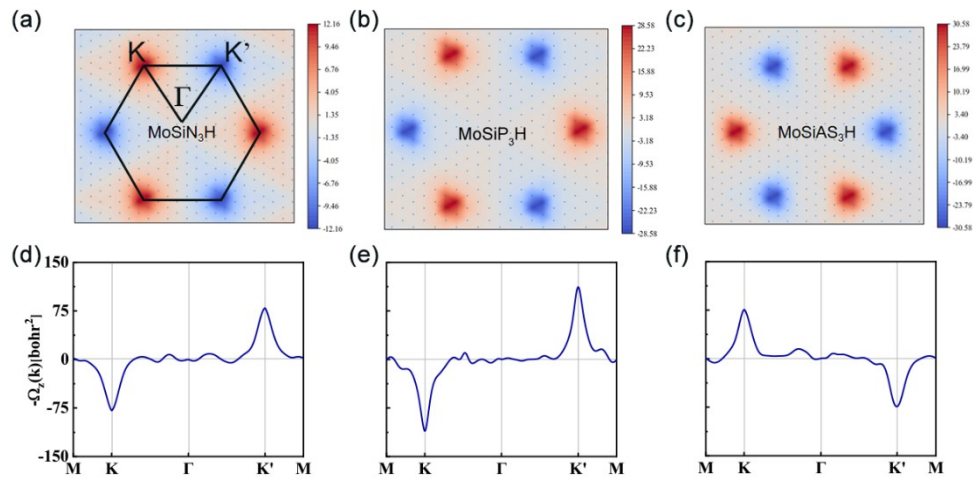
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[*] Address correspondence to E-mail: caixiaolin@hpu.edu.cn, jiayu@henu.edu.cn
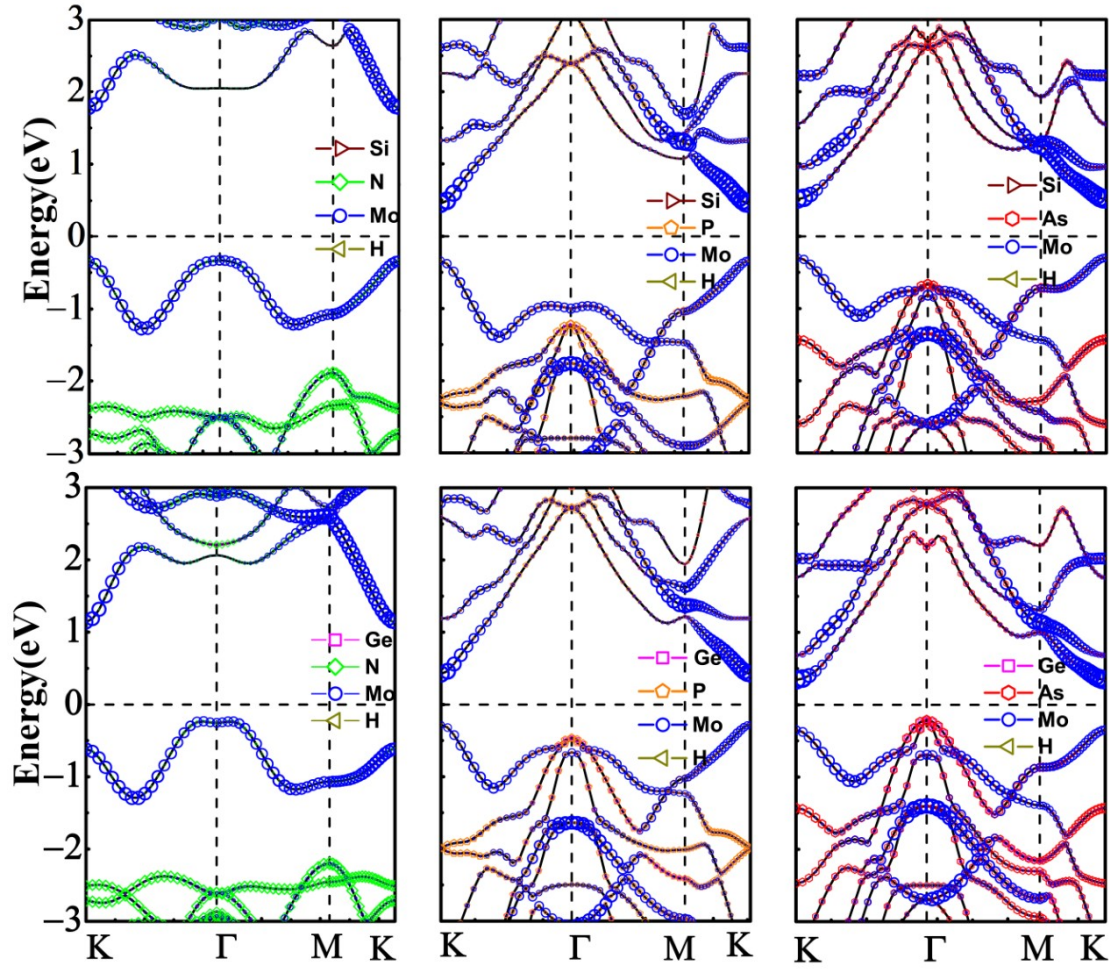
Fig. S1 The projection map of each atomic band structure of MoAZ$_3$H monolayer calculated by PBE function with Fermi level set to 0.
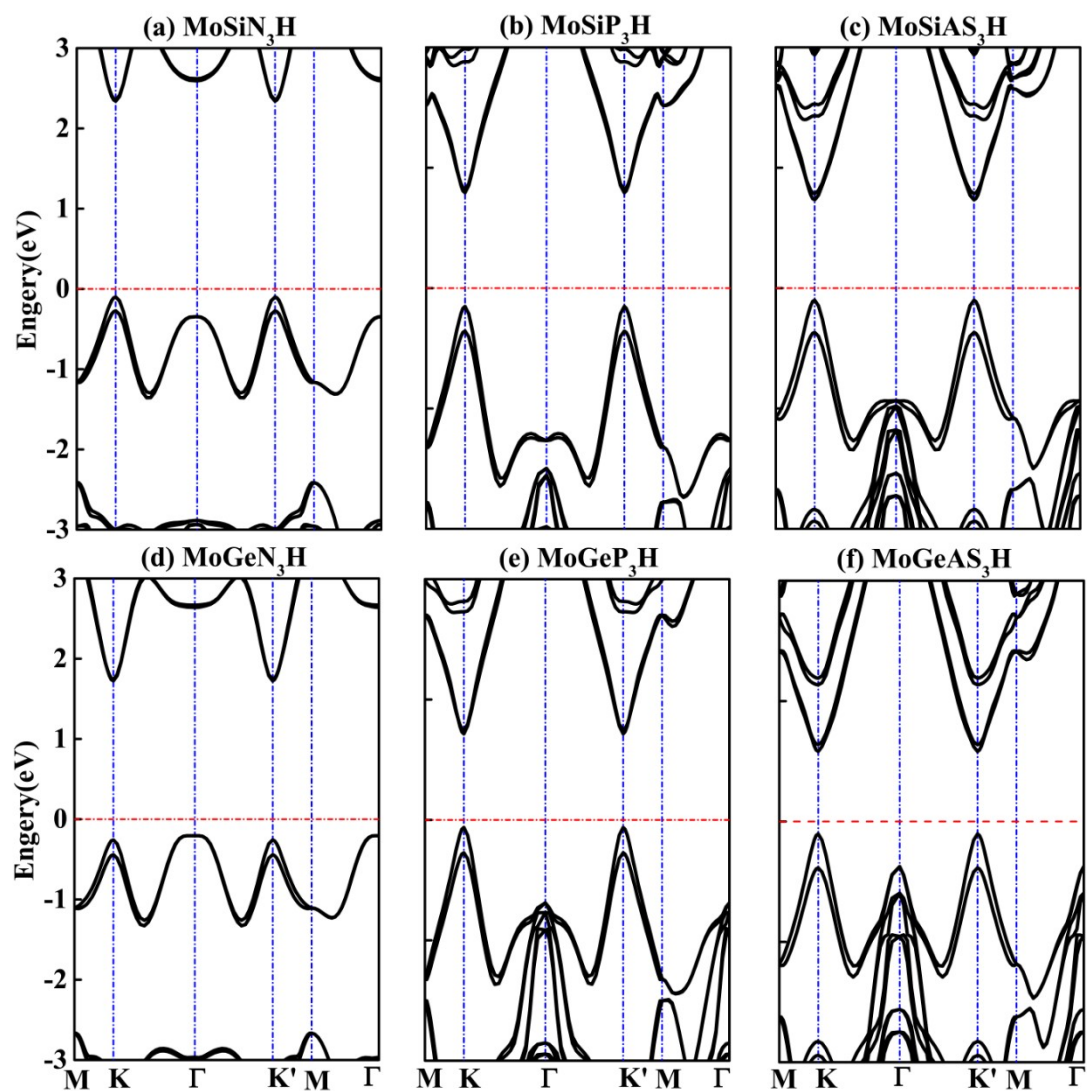
Fig. S2 Band structure diagram of MoAZ$_3$H monolayers calculated by HSE+SOC function, with Fermi energy level set to 0.

Fig. S3 (a)–(c) are Berry curvature diagrams of Janus MoSiA$_3$H (A = N, P, and As) ML in Brillouin zone. (d)–(f) are the corresponding Berry curvature curves along the high symmetry path.
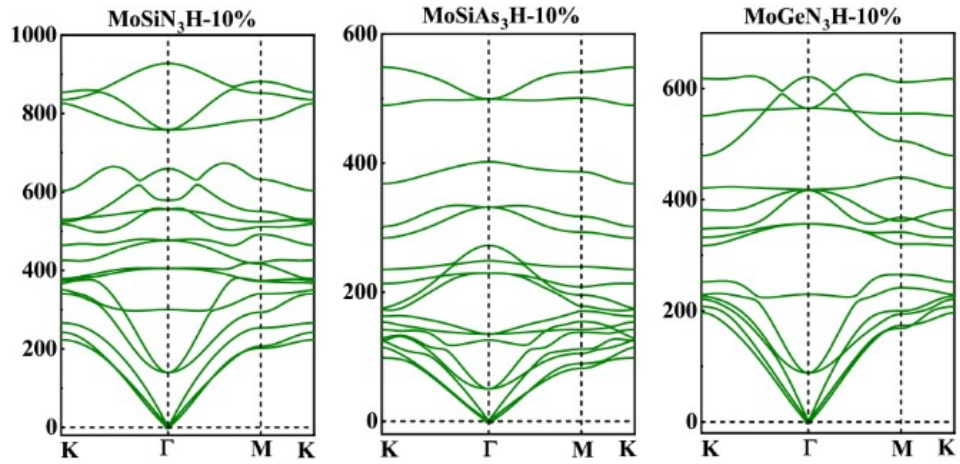
Fig. S4 Phonon spectra of the MoSiN$_3$H, MoSiAs$_3$H and MoGeN$_3$H under the tensile strain of 10%.