Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Materials

Janus $MoAZ_3H$ (A=Ge, Si; Z=N, P, As) monolayers: a new class of semiconductors exhibiting excellent photovoltaic and catalytic performances

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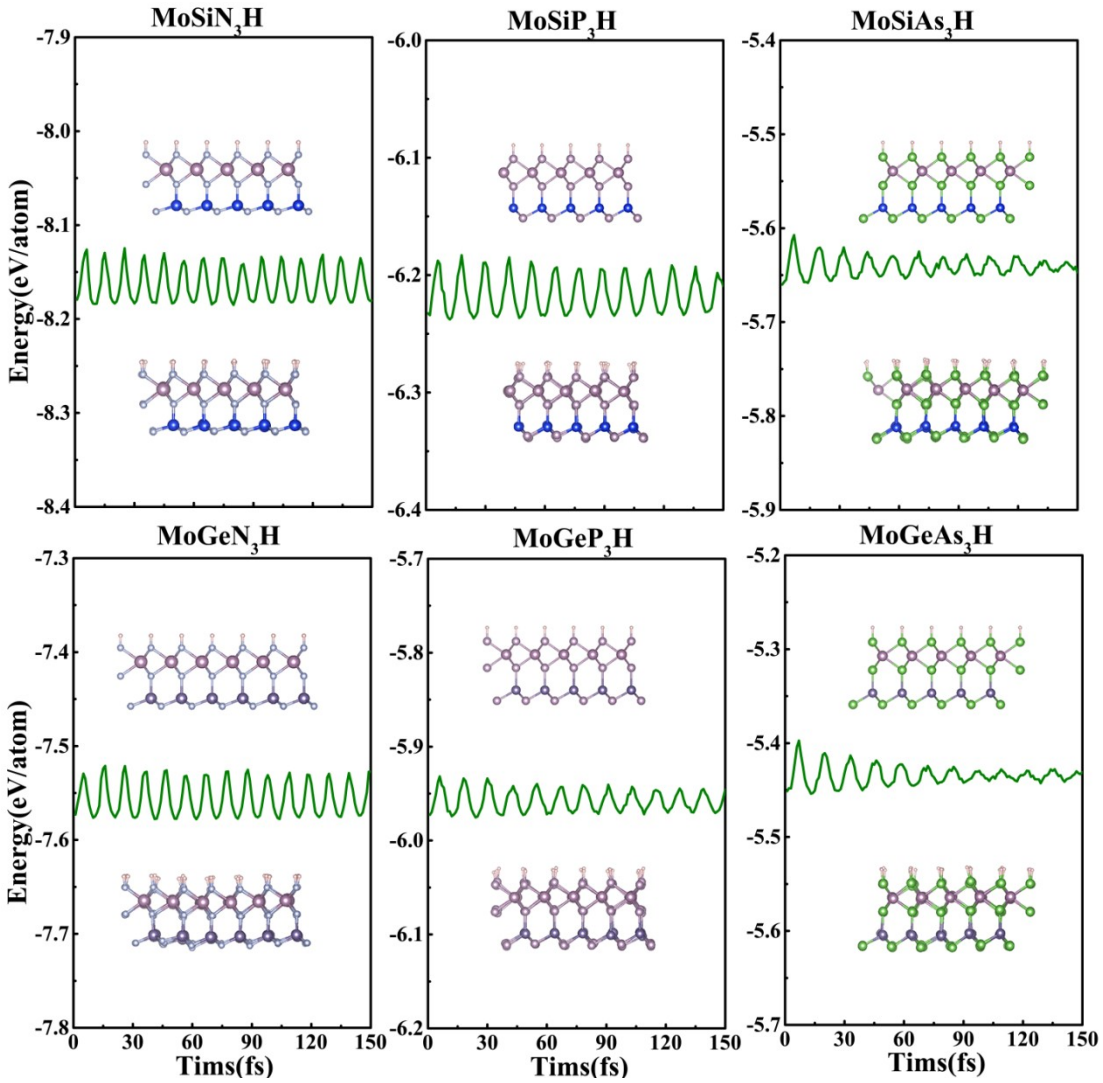

Fig. S1 AIMD simulation of $MoAZ_3H$ ML material, in which the green curve is the evolution of the energy per atom over time, and the top and bottom insets are the initial and final structures,

respectively.

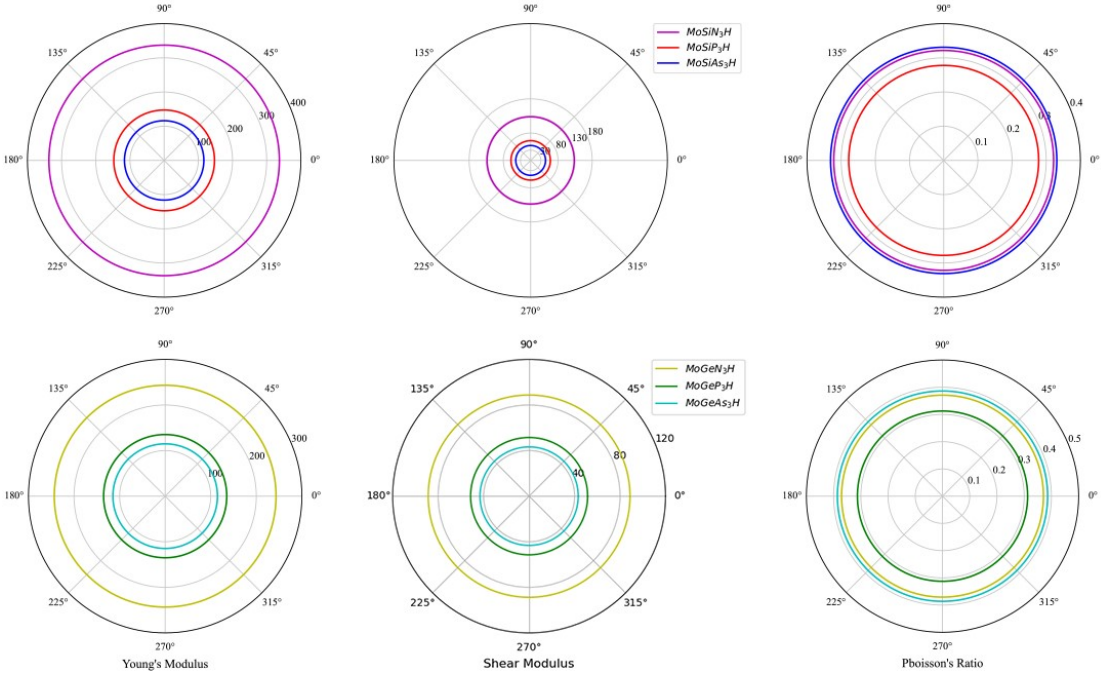

Fig. S2 Polar diagrams of Young's modulus, shear modulus and Poisson ratio of $MoAZ_3H$ ML.

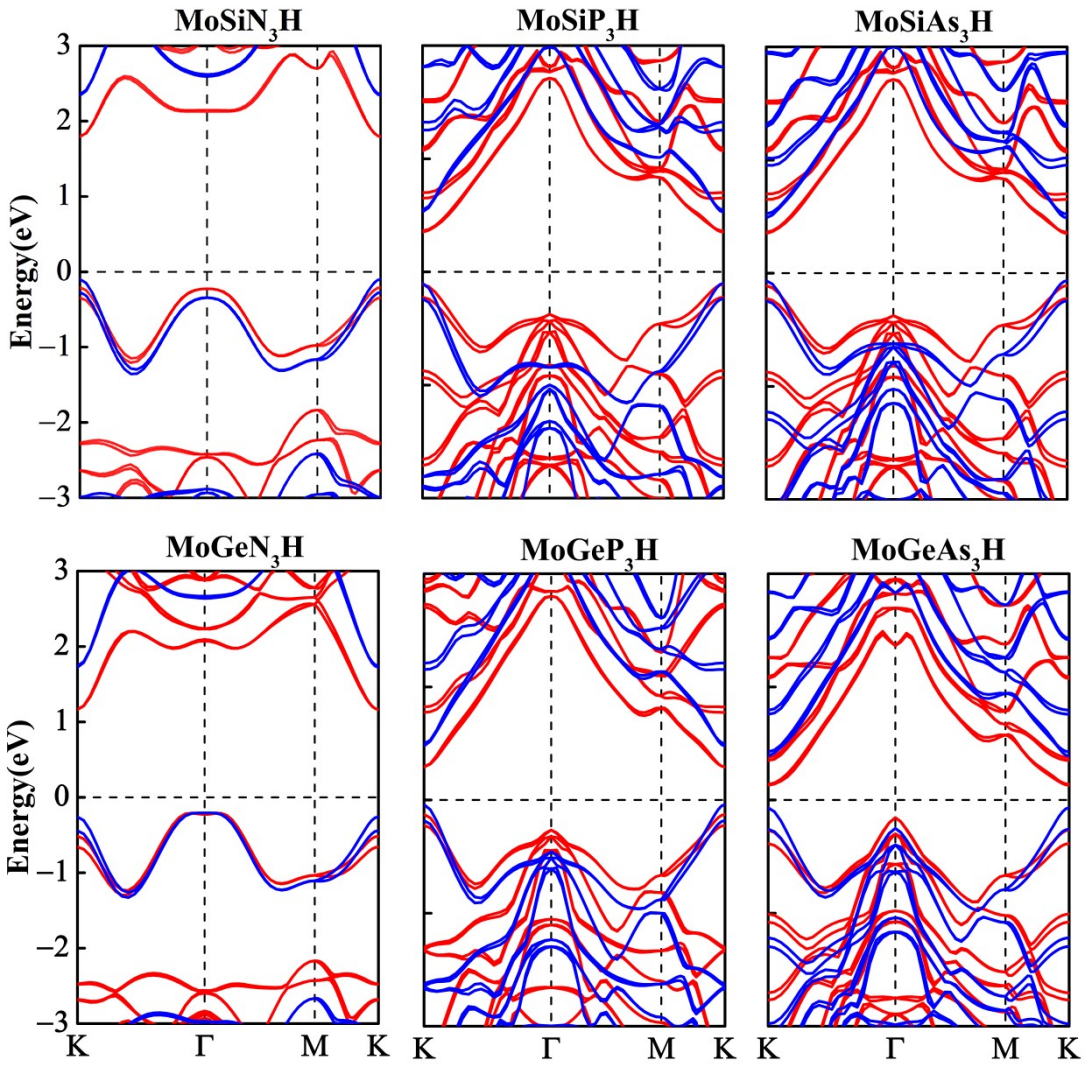

Fig. S3 Band structure diagram of $MoAZ_3H$ ML calculated by PBE+SOC (red lines) and HSE+SOC (blue lines) functionals, with Fermi energy level set to 0.

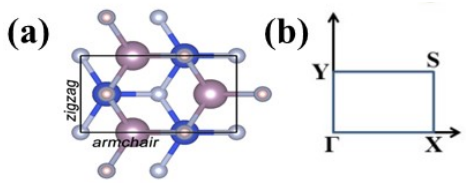

Fig. S4 (a) Top view of the rectangular unit cell and (b) the corresponding high symmetry path in the Brillouin zone for the $MoAZ_3H$ ML.

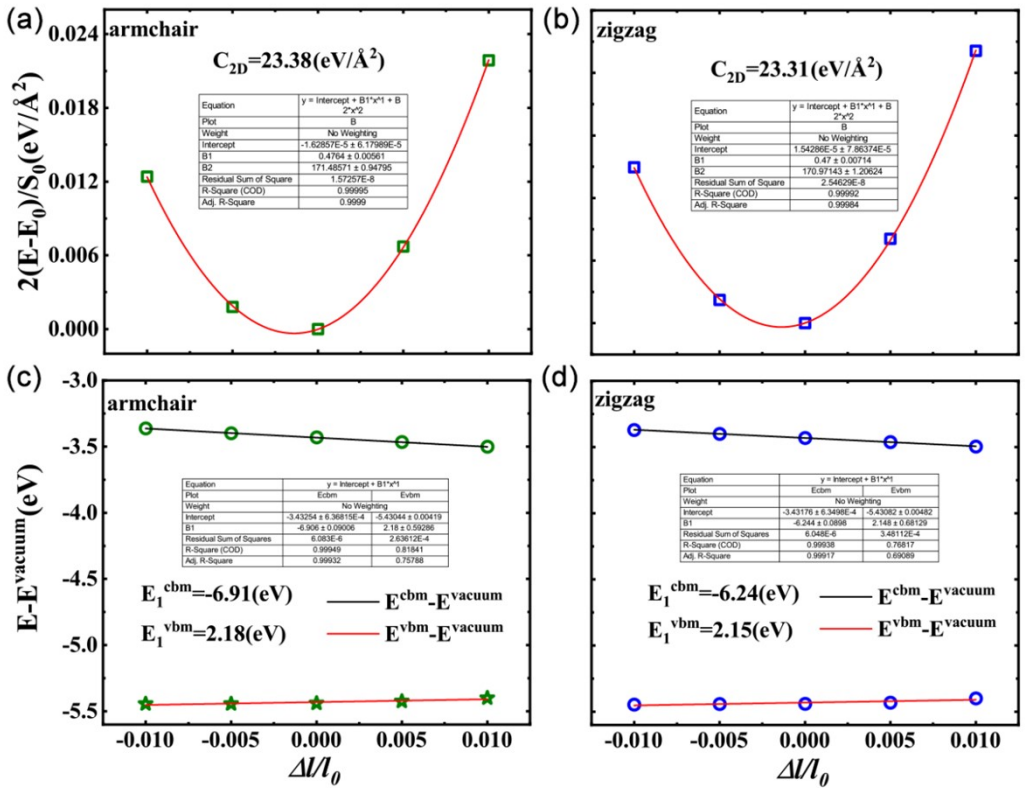

Fig. S5 In-plane stiffness and deformation potential of the $MoSiN_3H$ ML obtained from the PBE+SOC scheme.

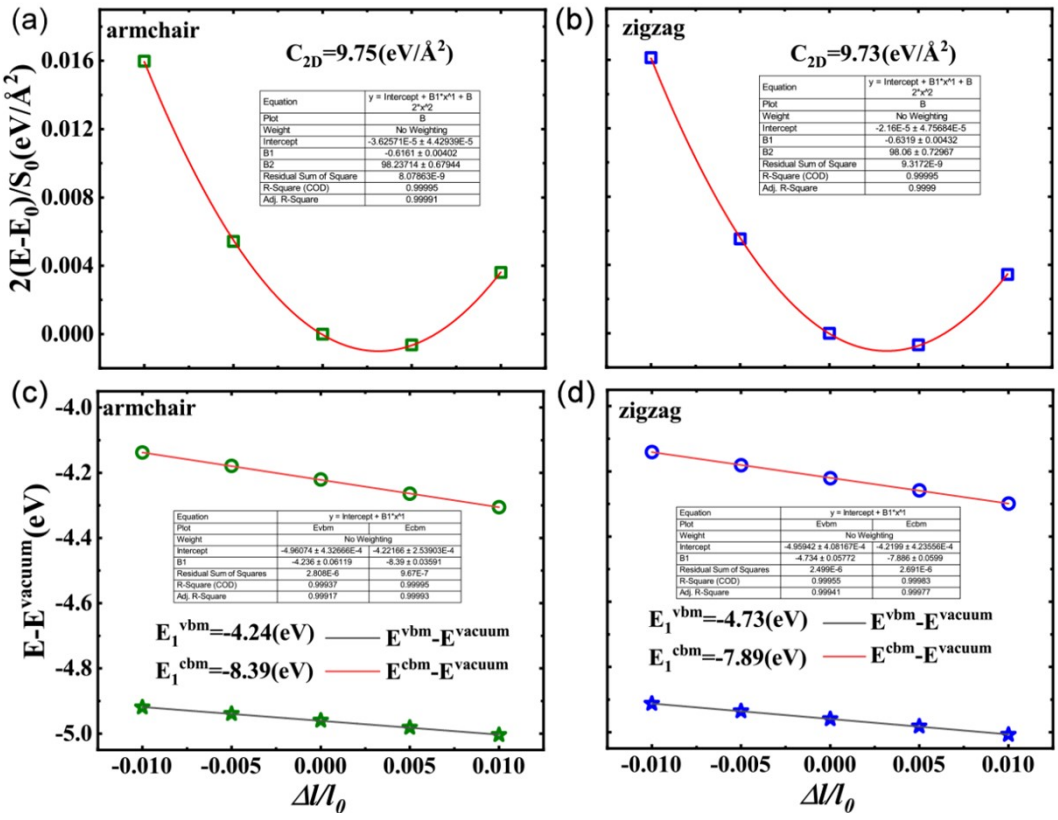

Fig. S6 In-plane stiffness and deformation potential of the $MoSiP_3H$ ML obtained from the PBE+SOC scheme.

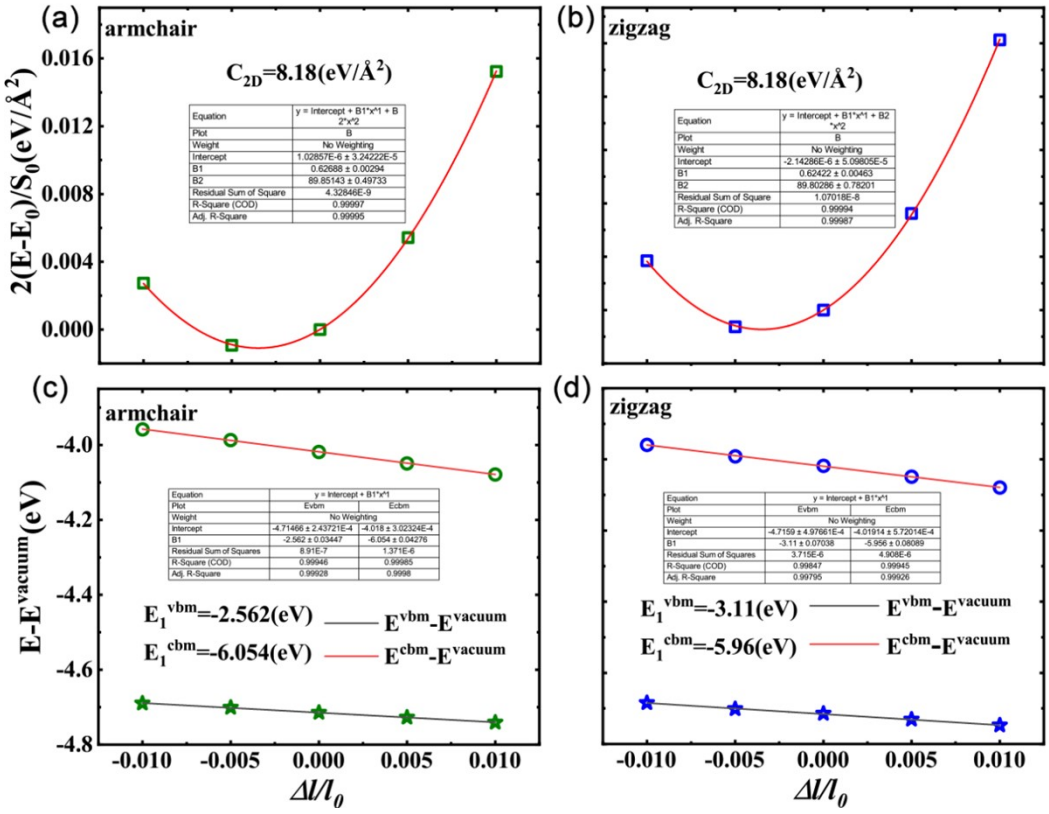

Fig. S7 In-plane stiffness and deformation potential of the $MoSiAs_3H$ ML obtained from the PBE+SOC scheme.

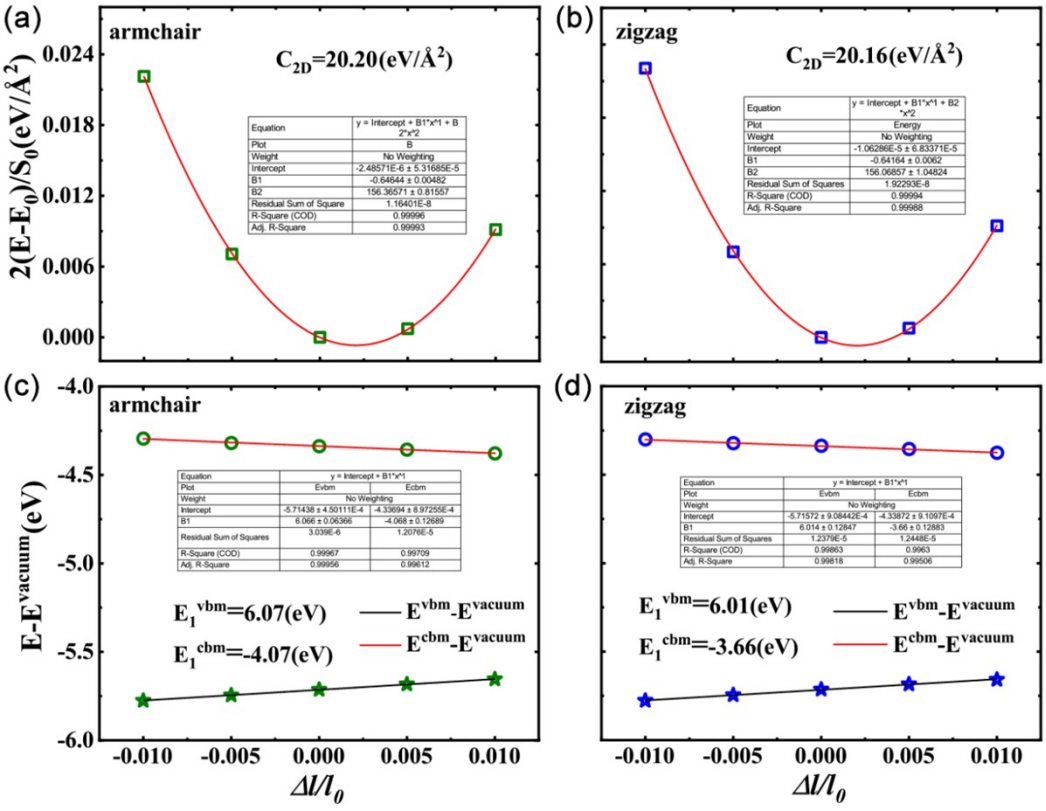

Fig. S8 In-plane stiffness and deformation potential of the $MoGeN_3H$ ML obtained from the PBE+SOC scheme.

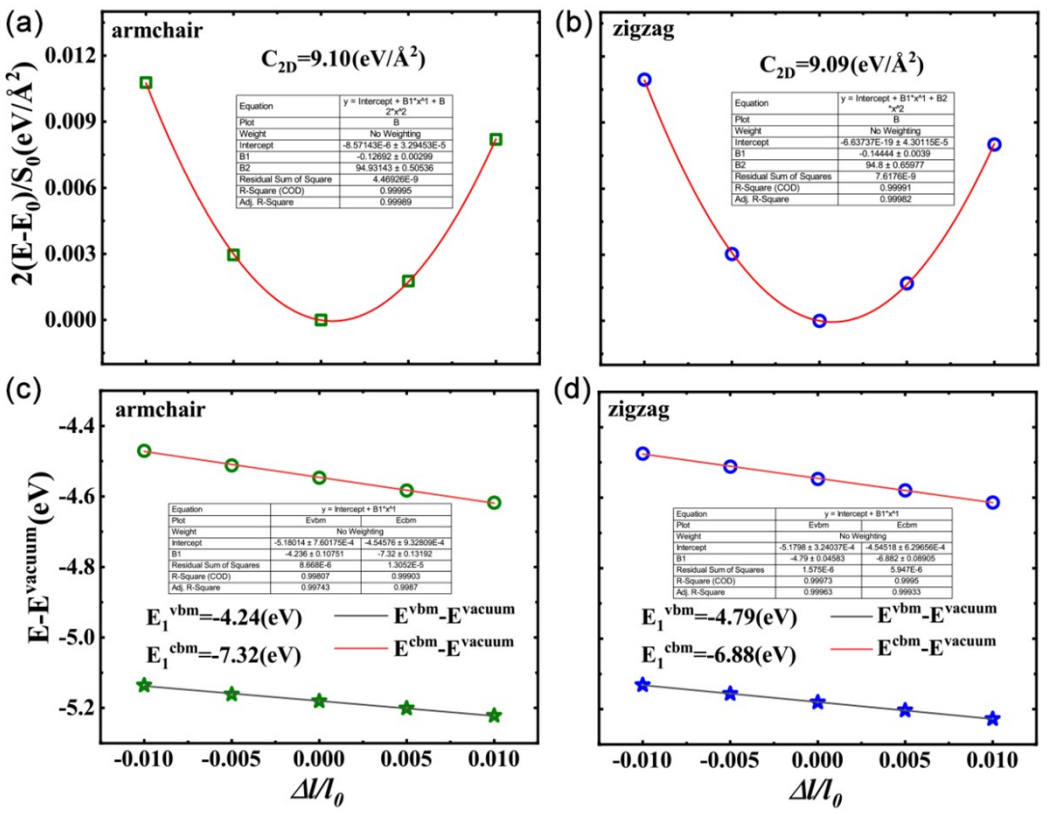

Fig. S9 In-plane stiffness and deformation potential of the $MoGeP_3H$ ML obtained from the PBE+SOC scheme.

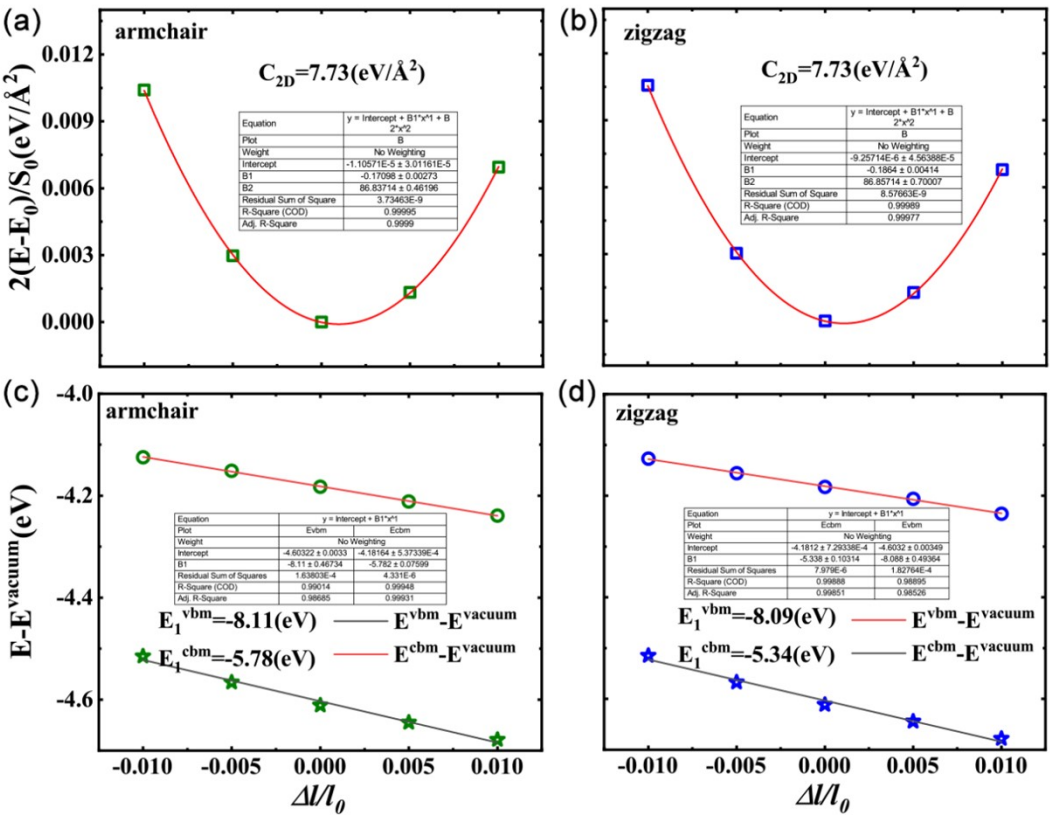

Fig. S10 In-plane stiffness and deformation potential of the $MoGeAs_3H$ ML obtained from the PBE+SOC scheme.