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

Flexible MA_2Z_4 (M= Mo, W; A= Si, Ge and Z=N, P, As) monolayers with outstanding mechanical, dynamical, piezoelectric properties and anomalous dynamic polarization

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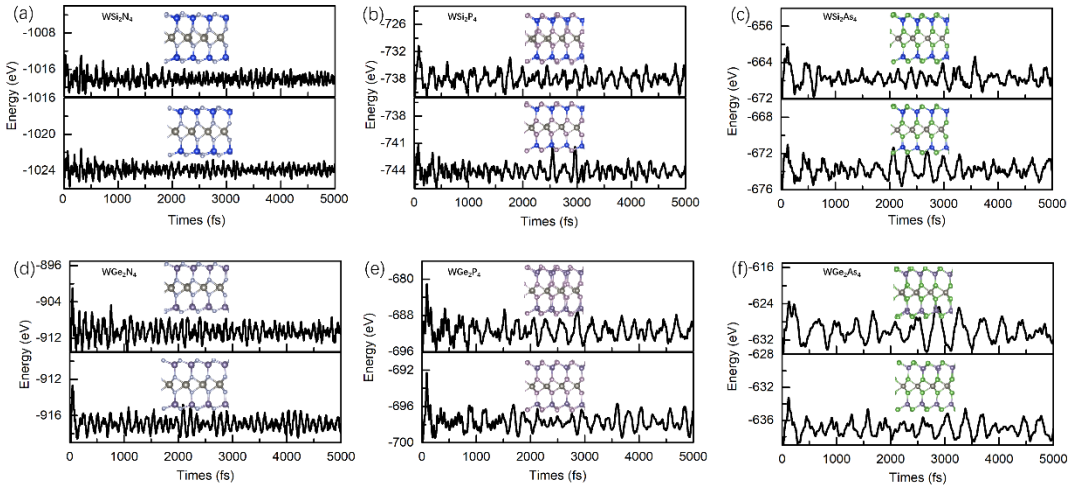

Fig.S1 (a) – (f) The evolution of the total energies and snapshot structures of WA_2Z_4 monolayers. The down and up variation in each picture represents simulations at 300 K and 700 K, respectively.

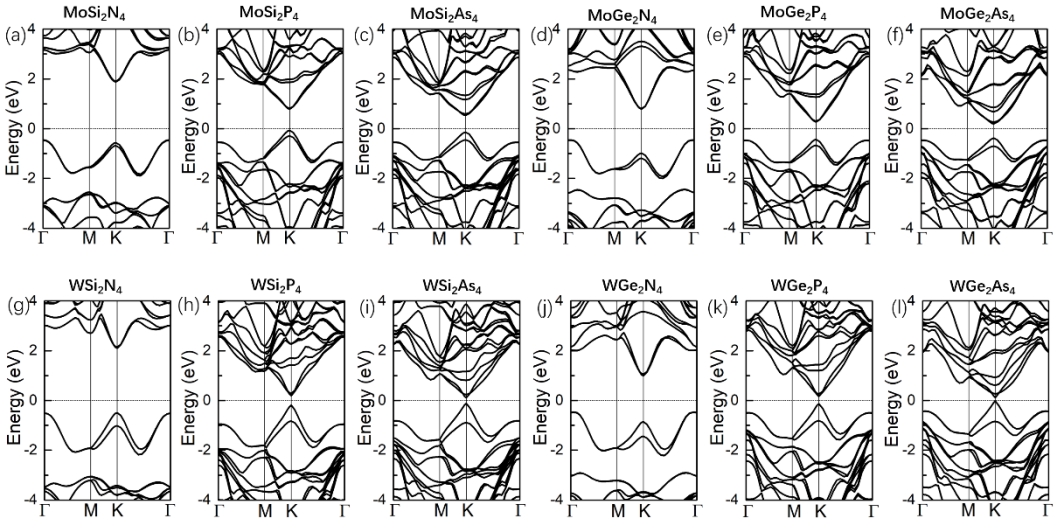

Fig. S2 (a)-(l) The band structures of MA_2Z_4 monolayers with HSE-SOC calculation

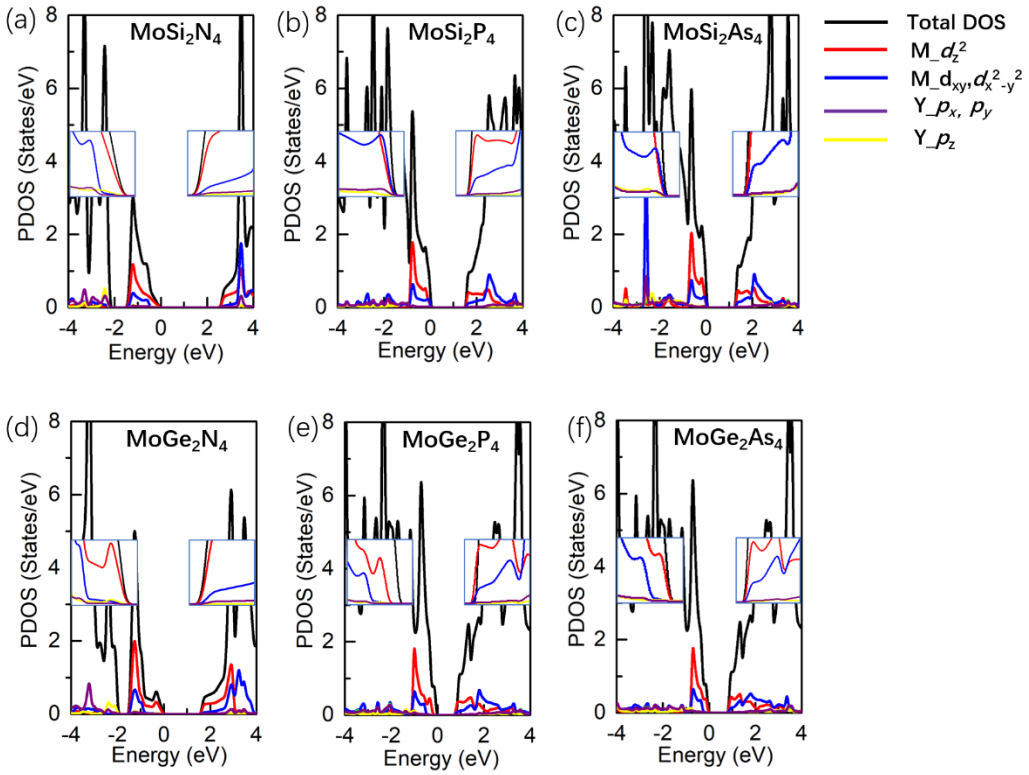

Fig. S3 (a) –(f) The projected density of states of MoA_2Z_4 monolayers with HSE calculation