Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

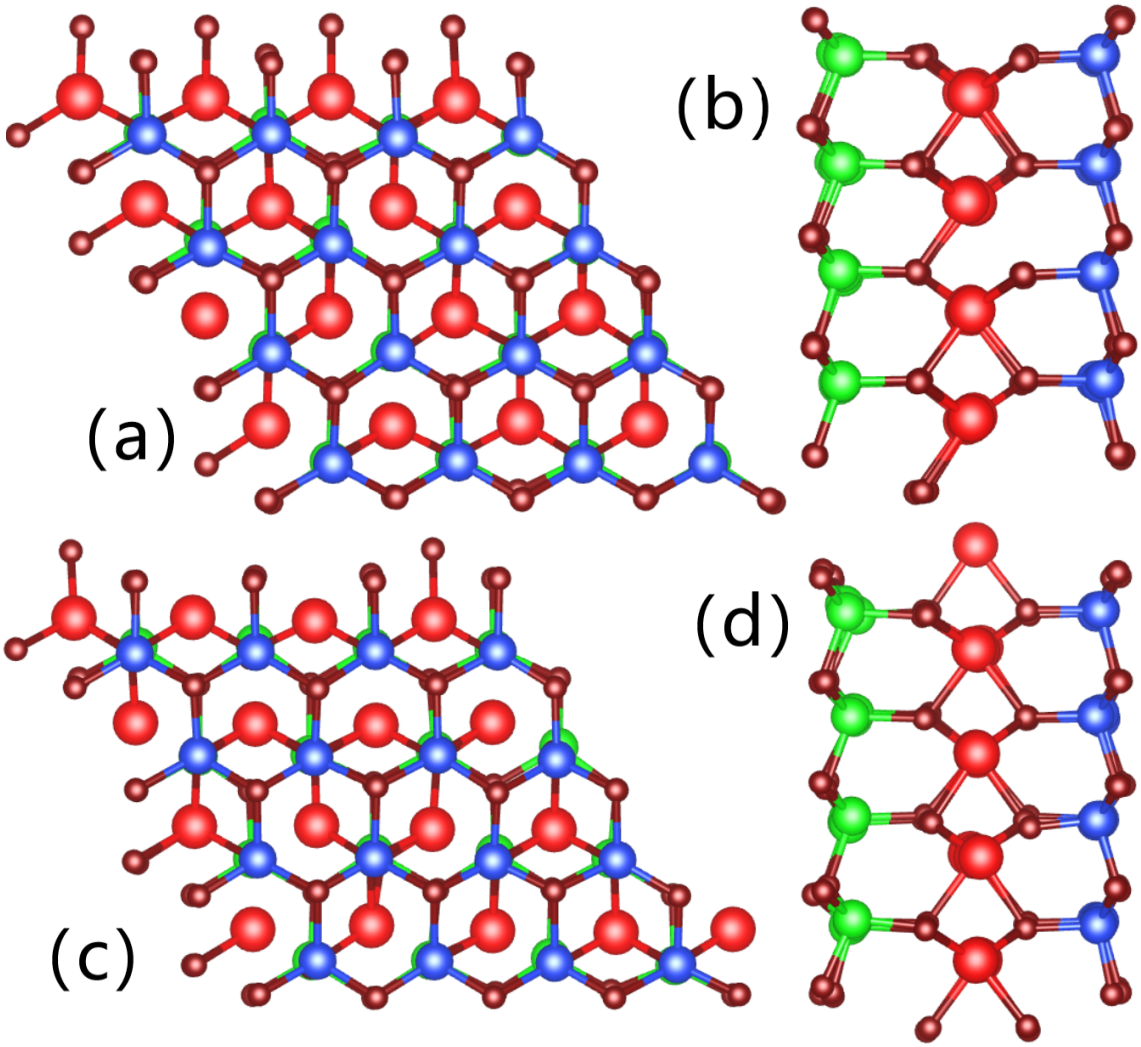

FIG. 1. (Color online) The crystal structures (a: Top views; b: Side views at 300 K and c: Top views; d: Side views at 600 K) of $WSiGeN_4$ after the simulation for 3 ps.

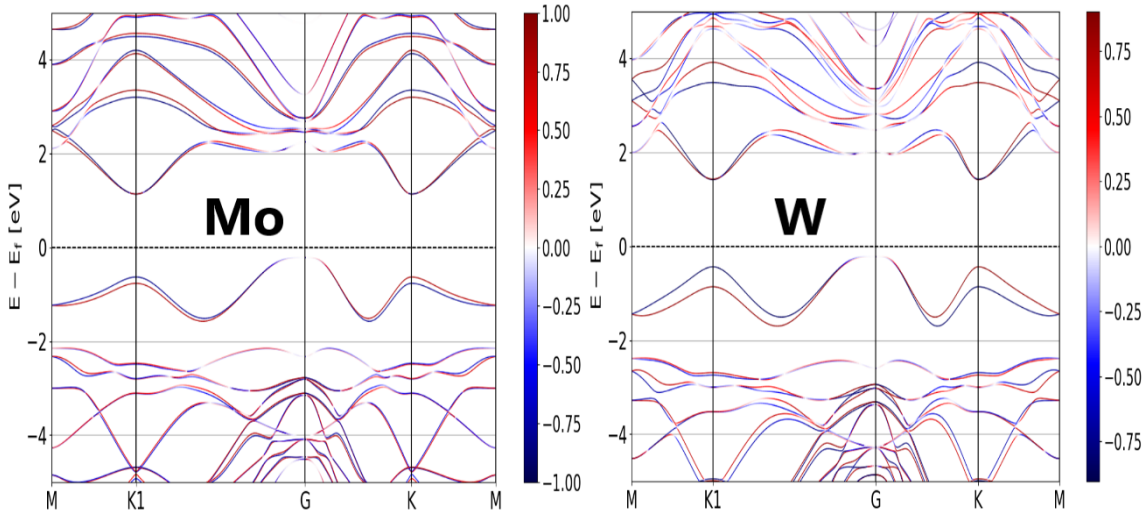

FIG. 2. (Color online) Band structures of monolayer $MSiGeN_4$ (M=Mo and W) monolayer in the presence of SOC along M (0, 0.5, 0)-K1 (-1/3, 2/3, 0)-G (0, 0, 0)-K (1/3, 1/3, 0)-M (0, 0.5, 0) high-symmetry path. The red and blue colors indicate the spin-up and spin-down bands, respectively.

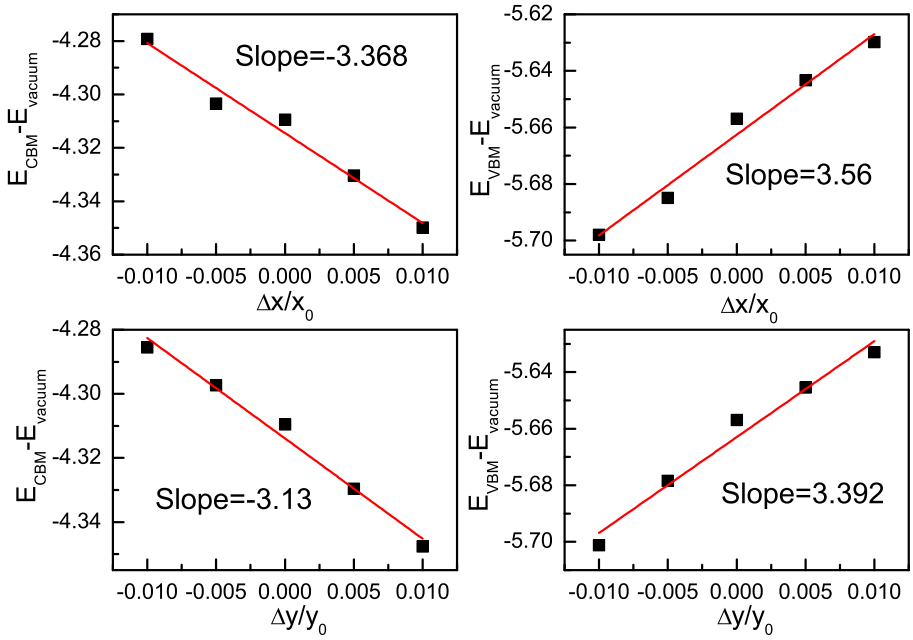

FIG. 3. (Color online)The band energies of the VBM and CBM of $MoSiGeN_4$ monolayer with respect to the vacuum energy as a function of lattice dilation along both x and y directions using GGA+SOC. The red solid lines are linear fitting curves with fitted slopes as the DP.

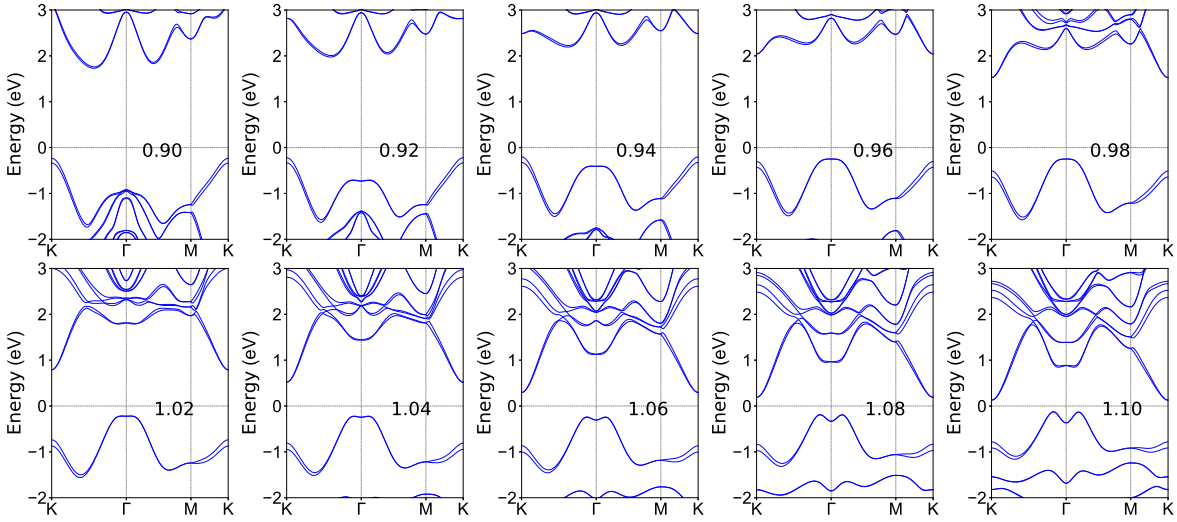

FIG. 4. (Color online) The energy band structures of $MoSiGeN_4$ monolayer using GGA+SOC with a/a_0 changing from 0.90 to 1.10.

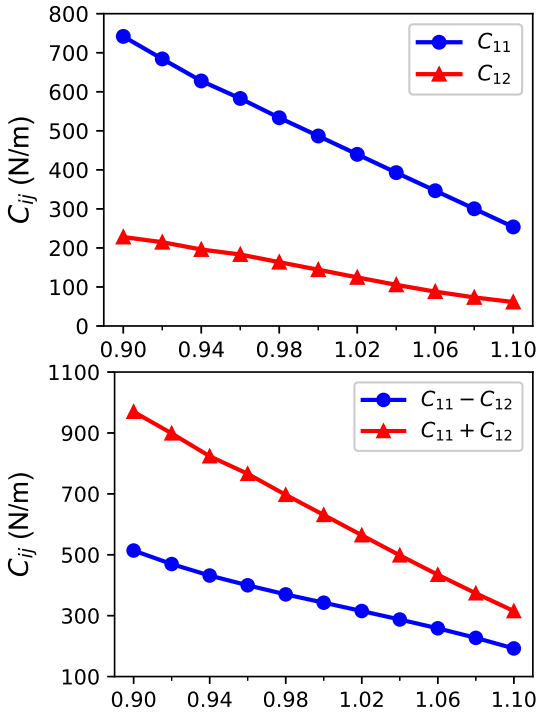

FIG. 5. (Color online) For monolayer $MoSiGeN_4$, the elastic constants C_{ij} with the application of biaxial strain (0.90 to 1.10).

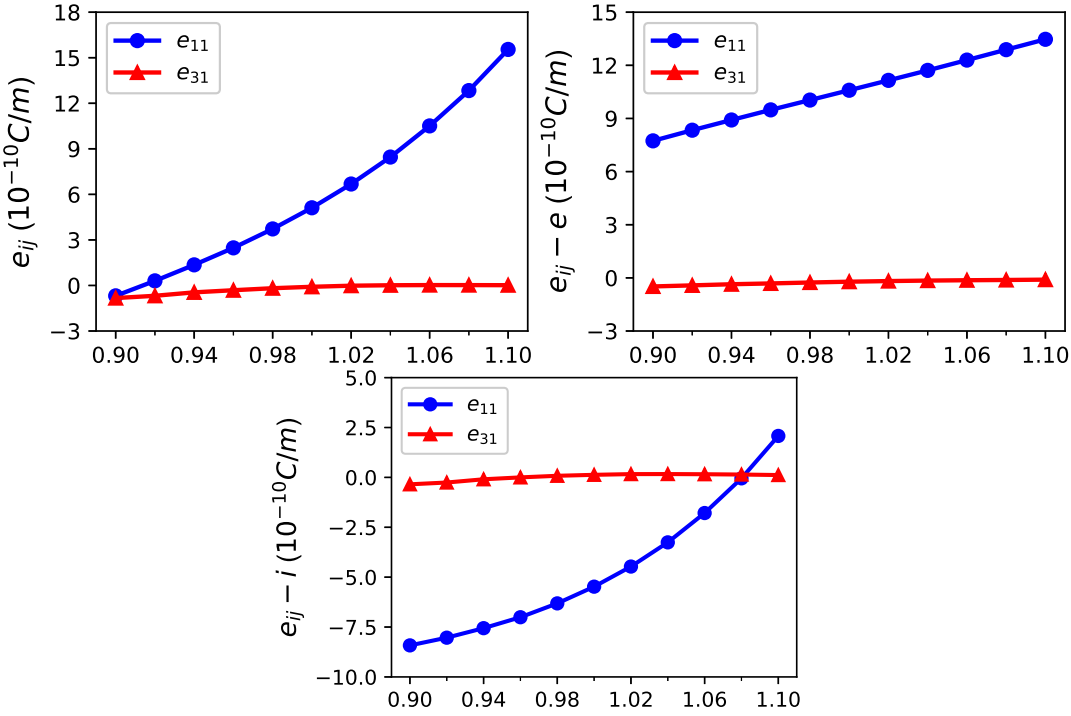

FIG. 6. (Color online) For monolayer $MoSiGeN_4$, the piezoelectric stress coefficients e_{11} and e_{31} along with the ionic contribution and electronic contribution to e_{11} and e_{31} with the application of biaxial strain (0.90 to 1.10).

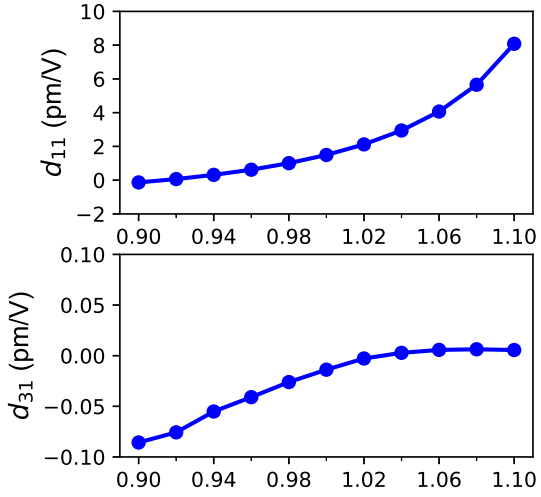

FIG. 7. (Color online) For monolayer $MoSiGeN_4$, the piezoelectric strain coefficients d_{11} and d_{31} with the application of biaxial strain (0.90 to 1.10).