Enhancing the magnetic properties (Curie temperature and magnetic anisotropy energy) of a 2D MXene (Ca_2C) by stacking a vdW heterostructure with silicene.

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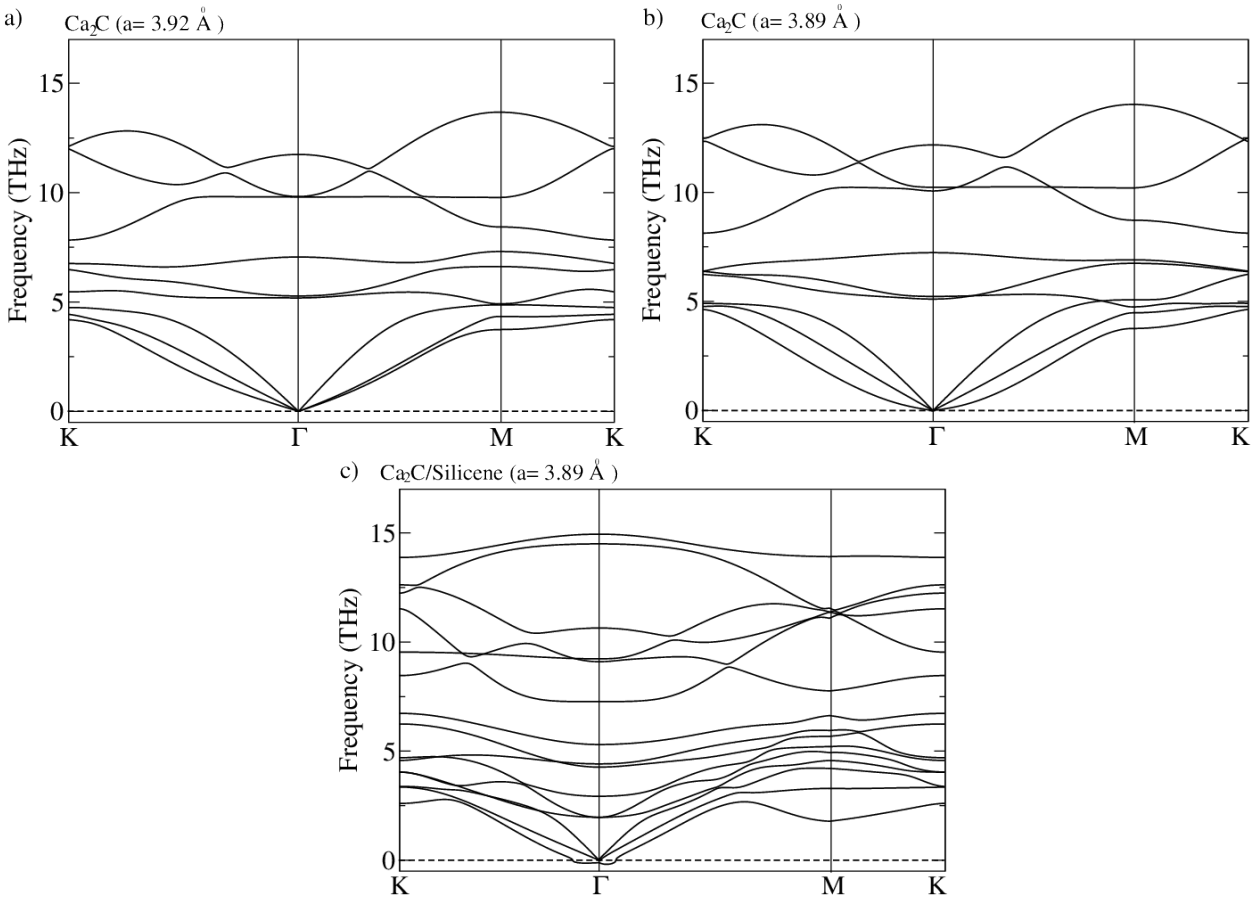

Figure 1: Calculated phonon spectrum: in a) Ca_2C optimized lattice parameter, b) Ca_2C in vdW lattice parameter and c) heterostructure vdW Ca_2C/silicene .

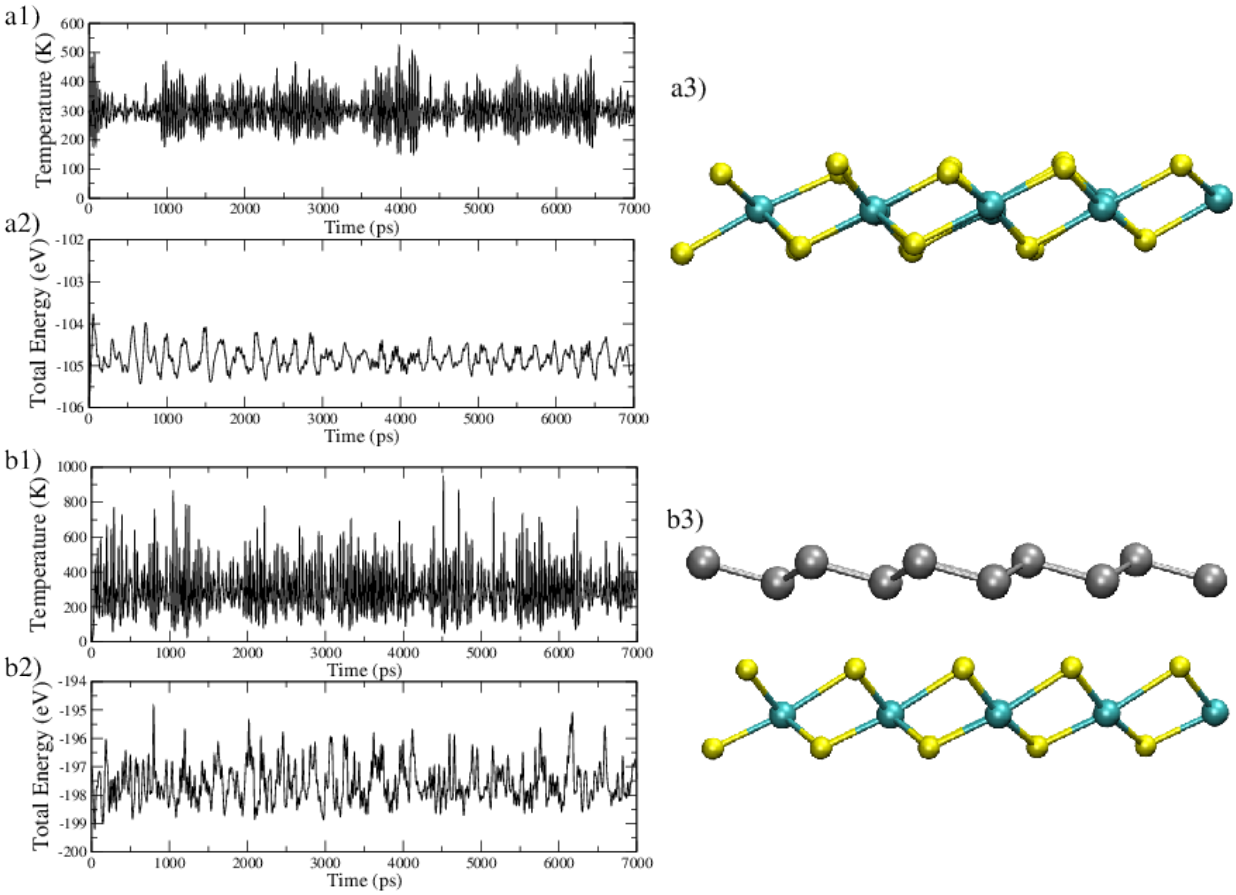

Figure 2: Molecular Dynamics calculations. Temperature and total energy as a function of the simulation time for the (a) Ca_2C monolayer and (b) Ca_2C/silicene van der Walls heterostructure, respectively.

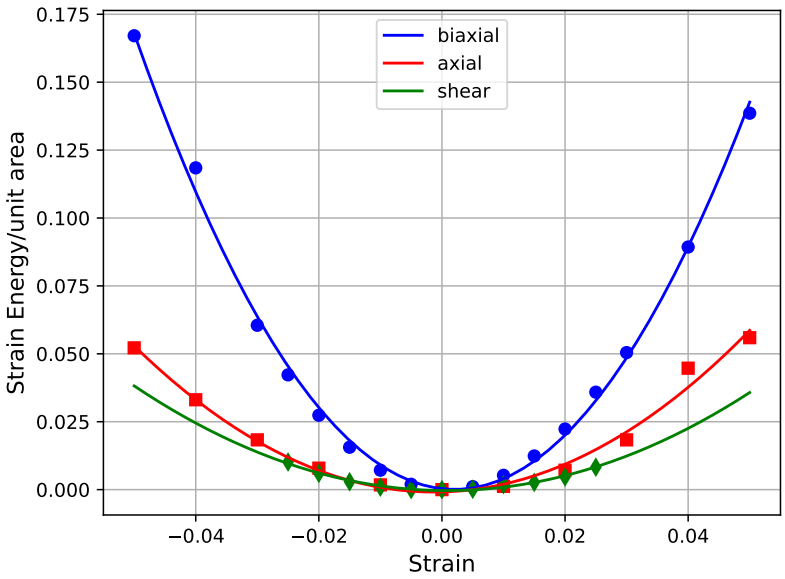

Figure 3: Calculated strain energy U(ε) as a function of the applied strain (ε).

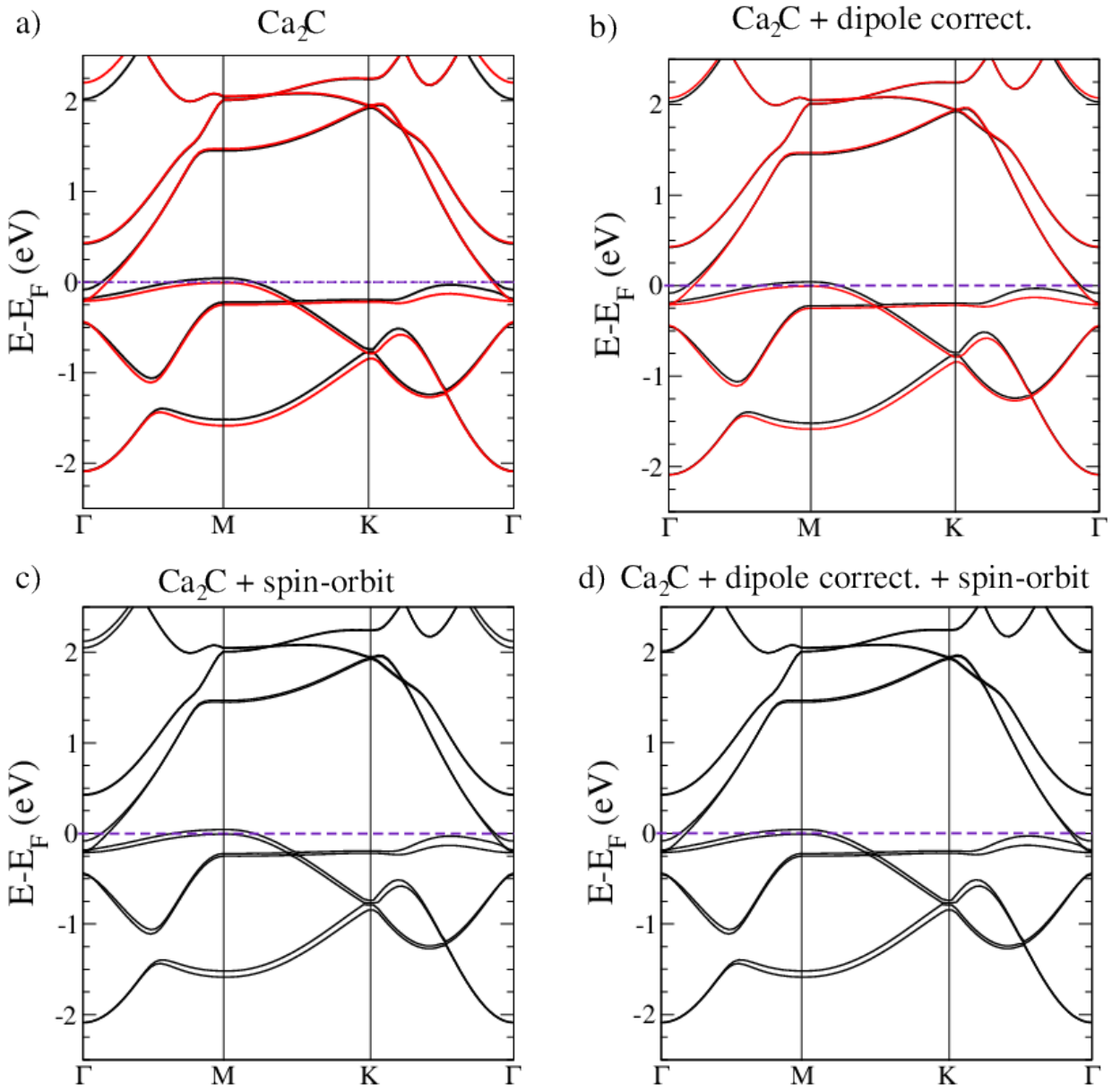

Figure 4: Calculated Electronic band structure for the Ca2C monolayer: (a) PBE; (b) PBE with electric dipole correction, (c) PBE + SOC and (d) PBE +SOC + Electric diploe correction.

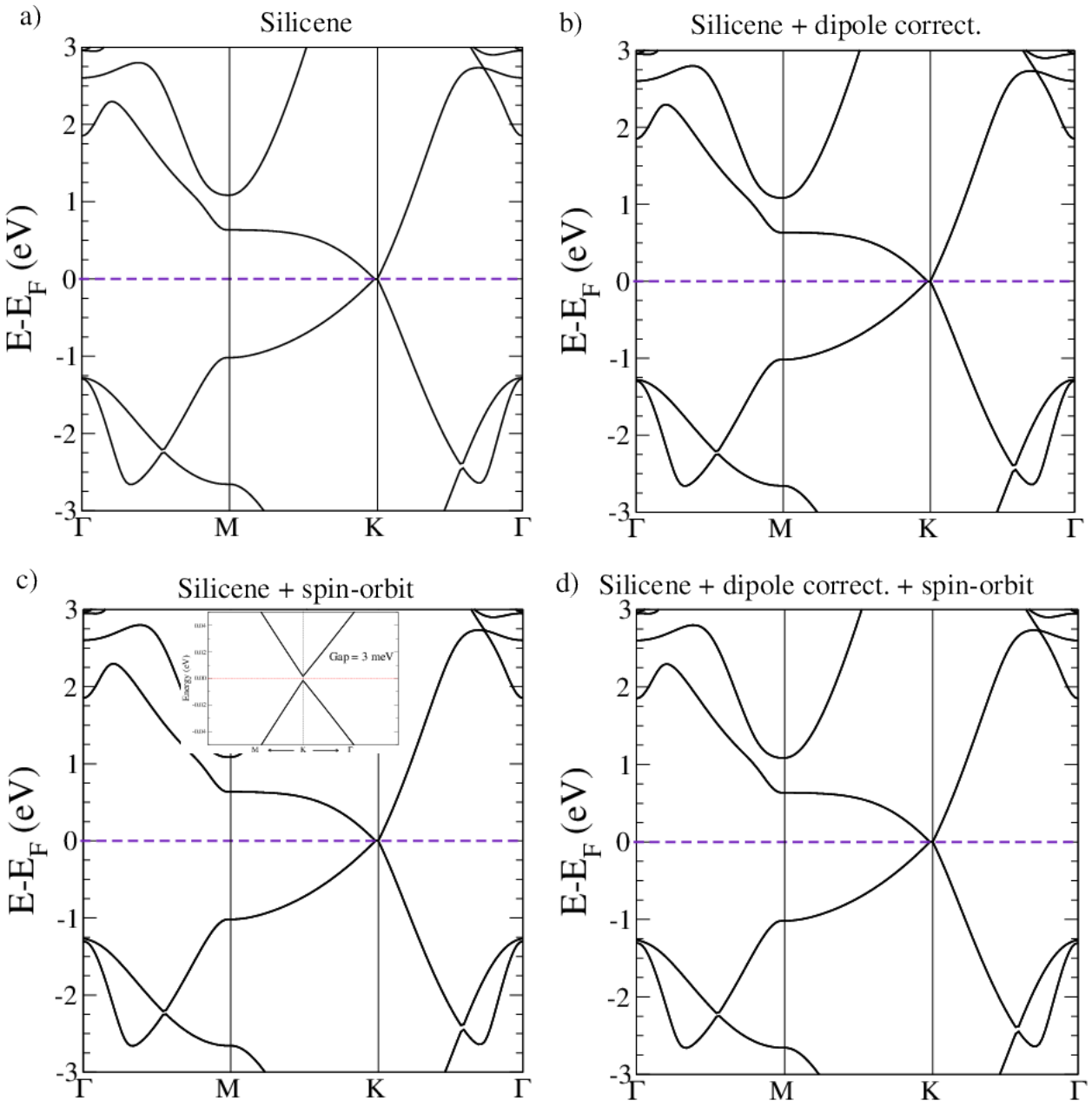

Figure 5: Calculated Electronic band structure for silicene: (a) PBE; (b) PBE with electric dipole correction, (c) PBE + SOC and (d) PBE +SOC + Electric dipole correction.

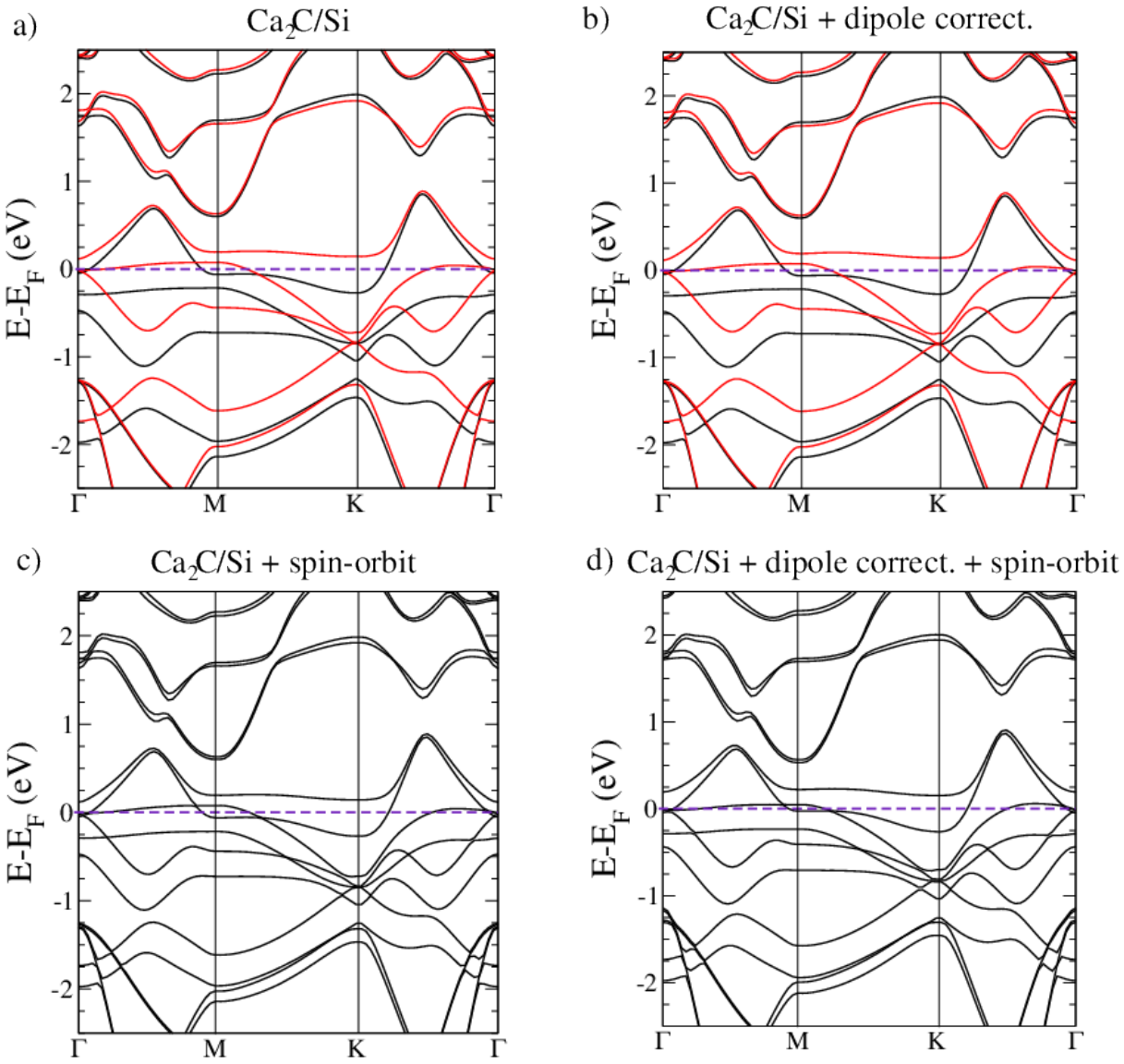

Figure 6: Calculated Electronic band structure for the vdW heterostructure (Ca2C/silicene): (a) PBE; (b) PBE with electric dipole correction, (c) PBE + SOC and (d) PBE +SOC + Electric dipole correction.

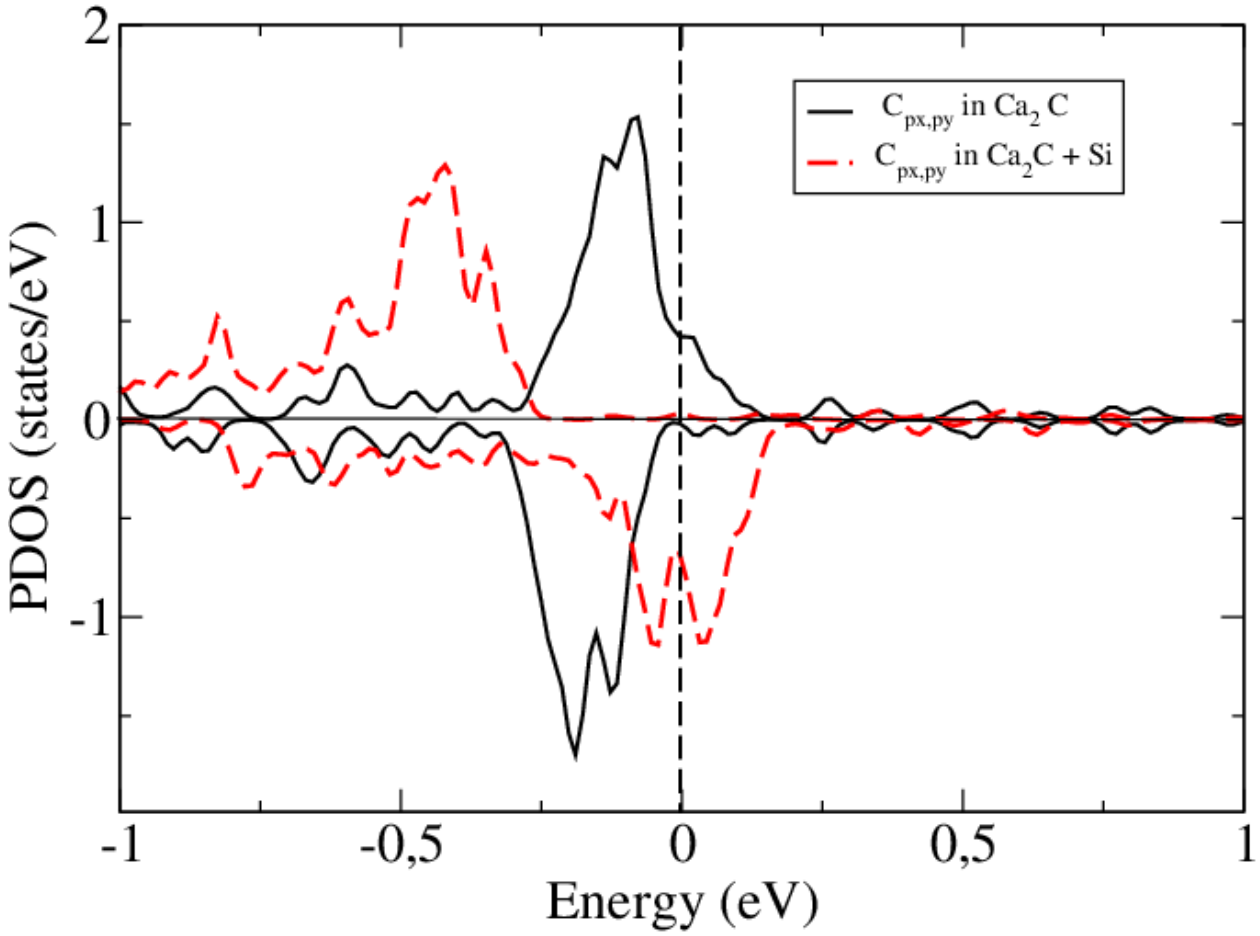

Figure 7: Projected Density of States for planar (p_x and p_y) orbitals of the carbon in the Ca_2C and Ca_2C/silicene vdW heterostructure.

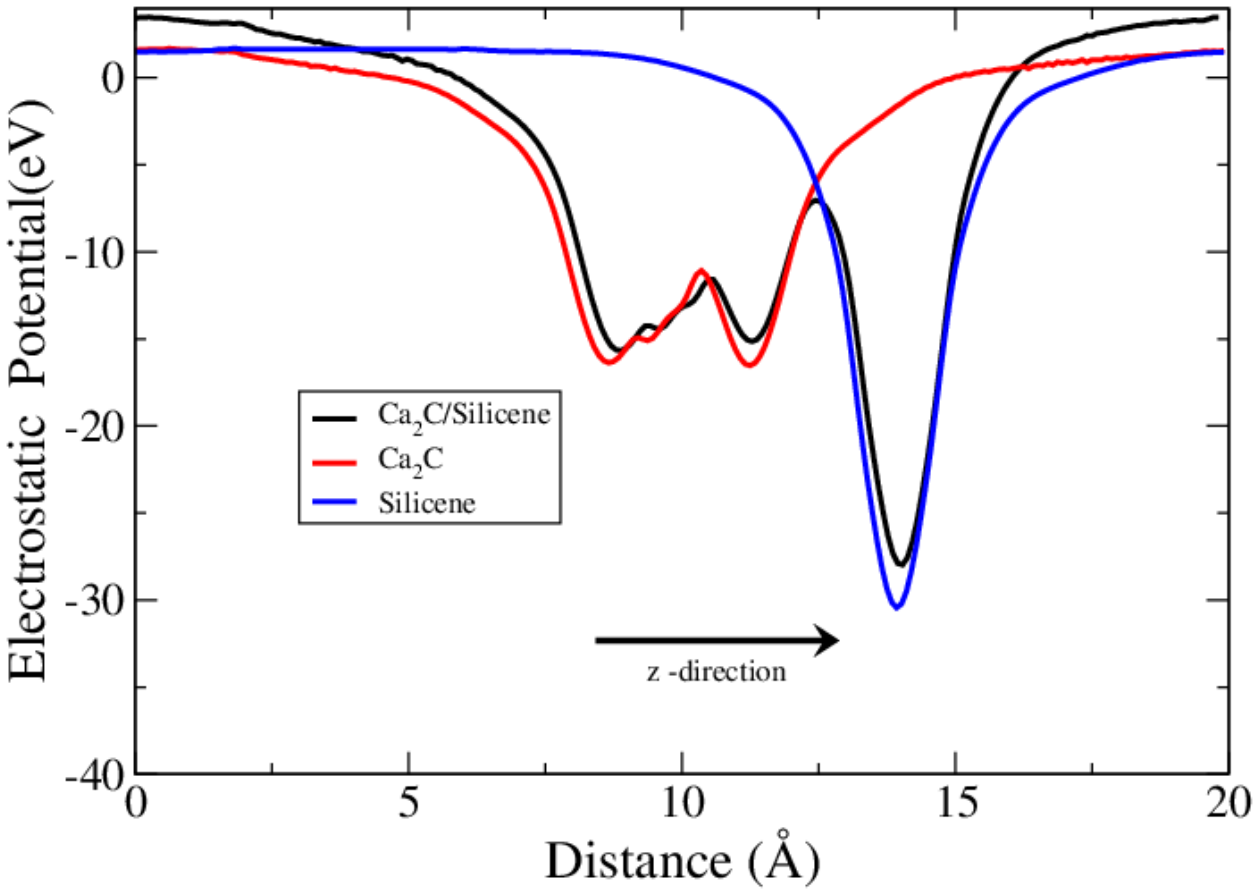

Figure 8: Calculated Electrostatic potentials of silicene, Ca_2C, and Ca_2C/silicene heterostructure.

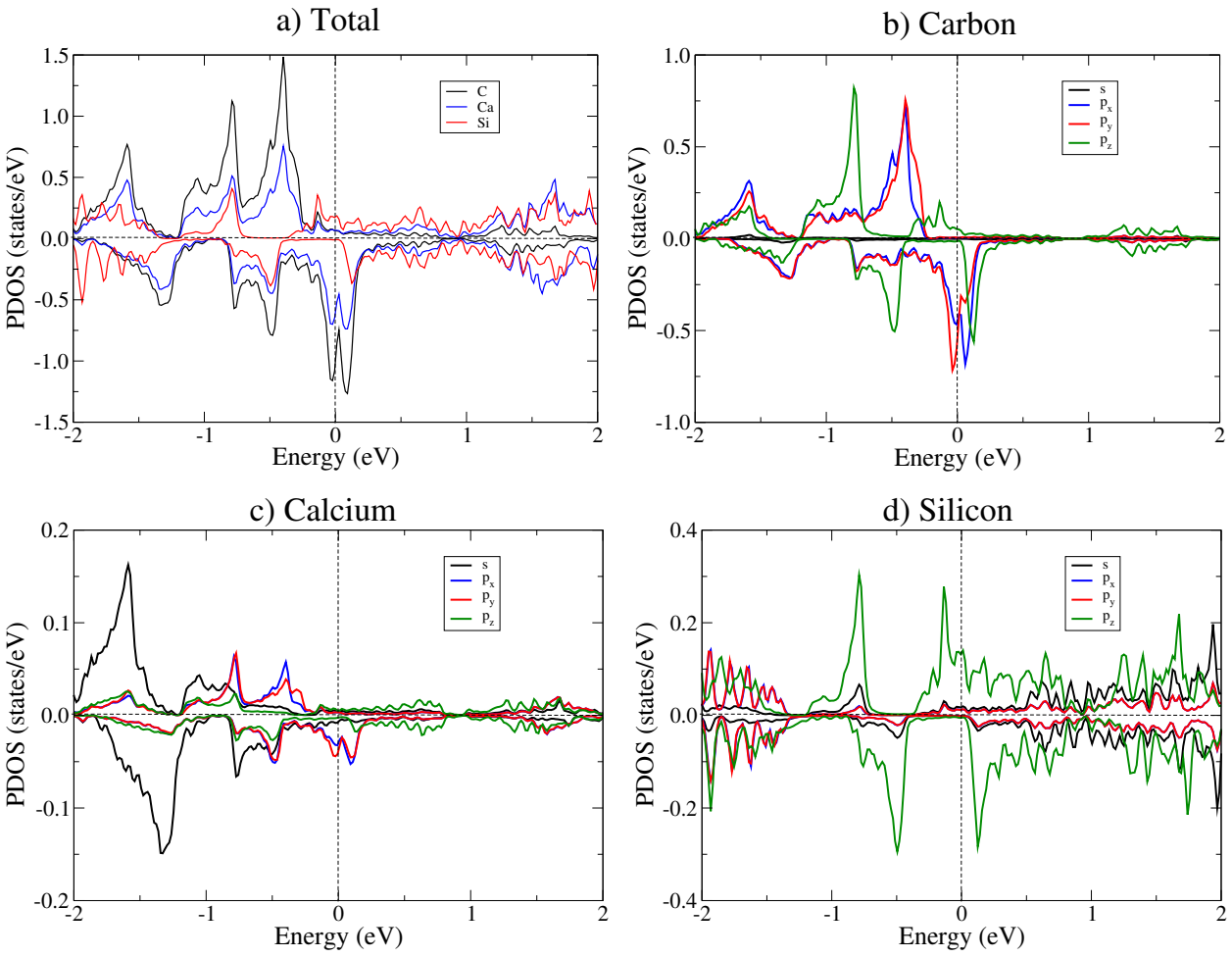

Figure 9: Projected Density of States: (a) on the atomic species; (b)-(d) on the atomic orbital for the C, Ca and Si atomic, respectively.

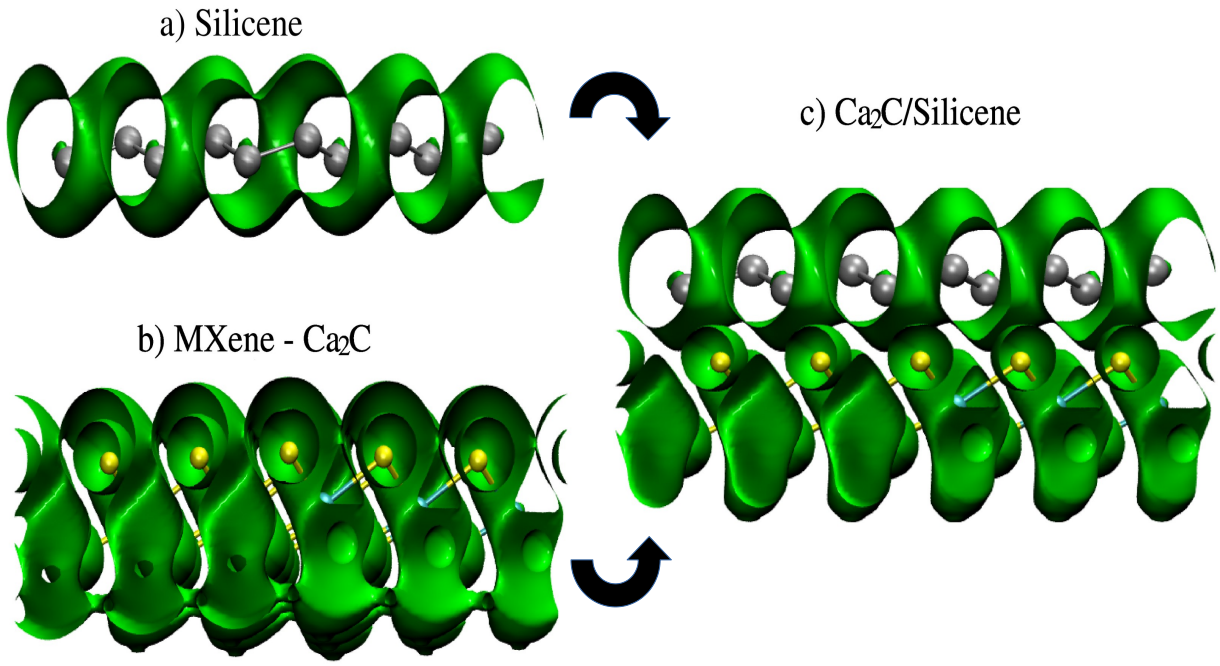

Figure 10: Electron Localization Function (ELF) for a) Silicene, b) Ca_2C and in c) Ca_2C/Silicene vdW heterostructure.The isovalue used was 0.1 $e\mathring{A}^{-3}$.

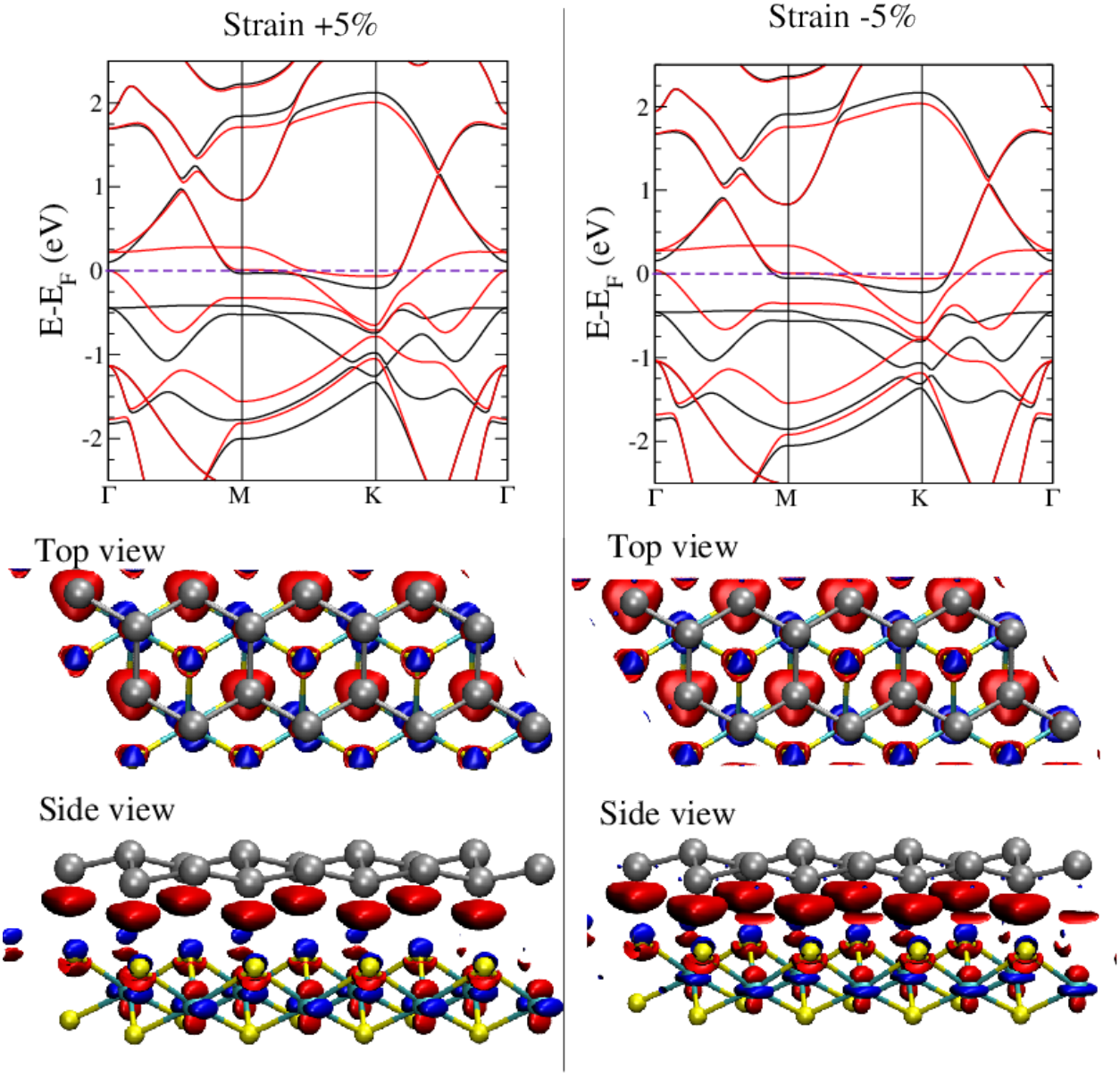

Figure 11: Electronic band structure and electronic charge difference for the Ca_2C/Silicene vdW heterostructure with vertical strain (ε_h) of $\pm$ 5 %). The isovalue used was 0.025 $e\mathring{A}^{-3}$.

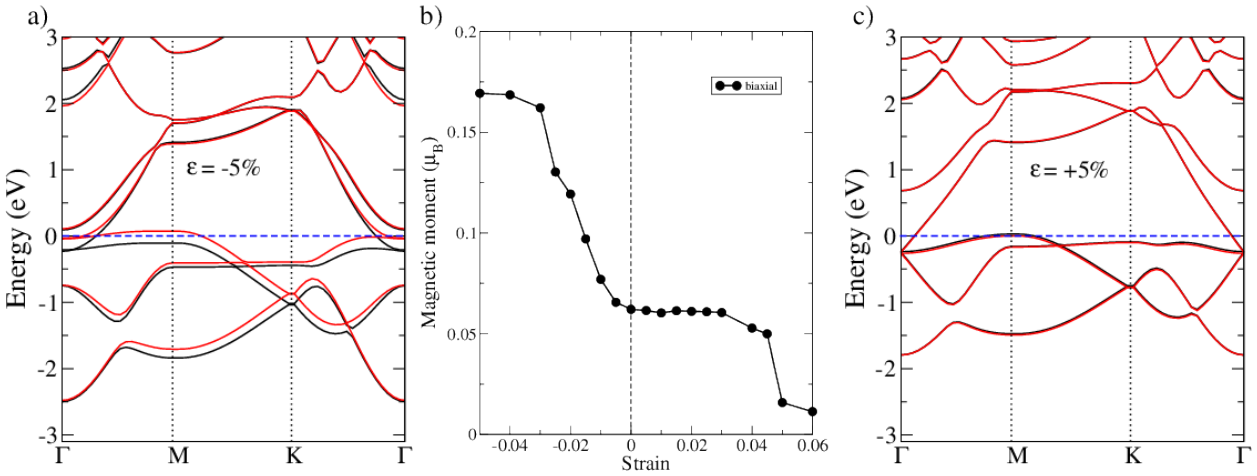

Figure 12: Electronic band structure [(a) and (c)] of the Ca_2C monolayer under planar biaxial strain ($\varepsilon = \mp 5$ %) and (b) magnetic moment as a function of strain.