

Supplementary Material

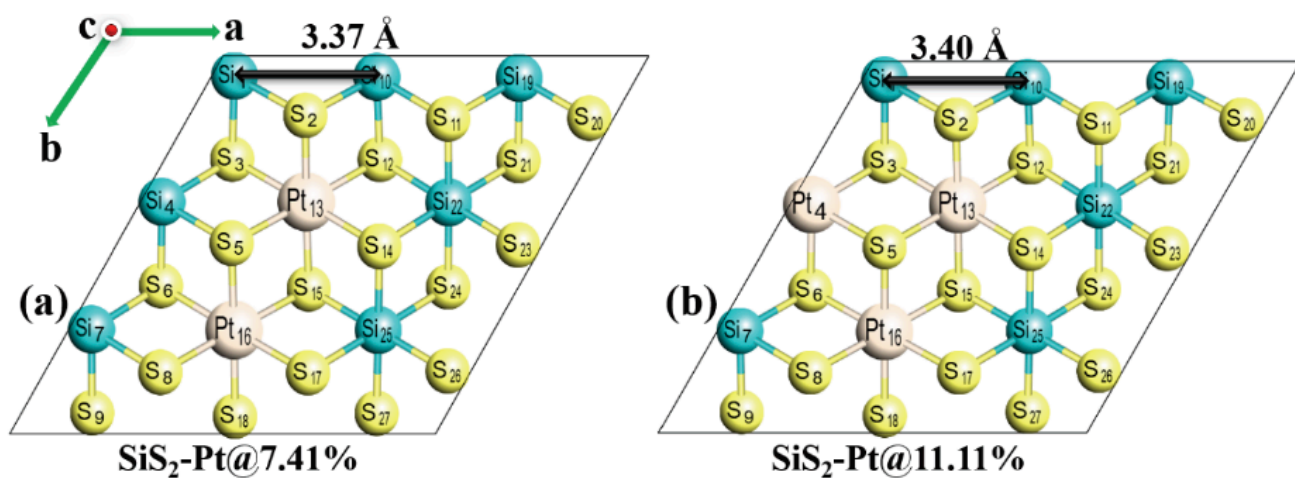


Figure S1: Showing the increase in the lattice constant with the increased percentage doping concentration. (a) two and (b) three Pt-atom doped SiS_2 monolayer, respectively.

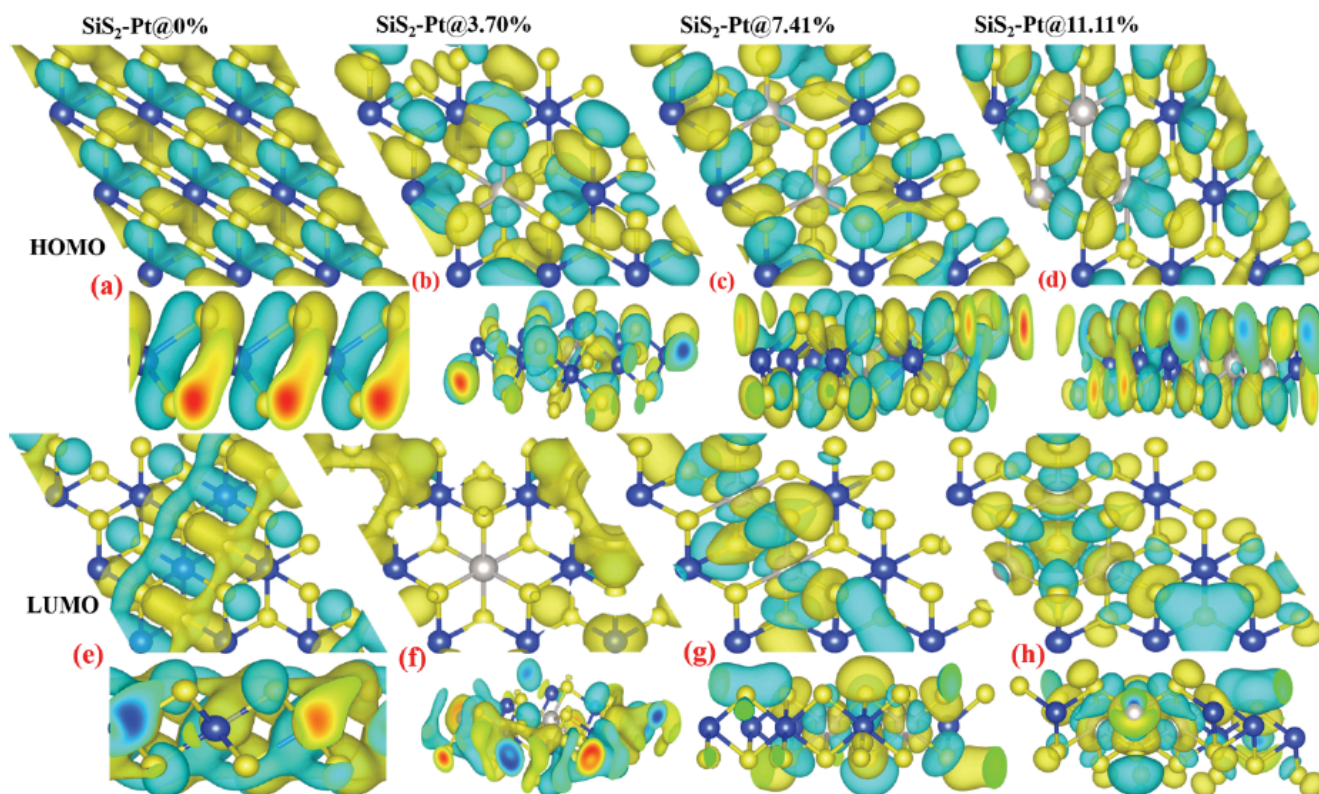


Figure S2: Frontier molecular orbitals of pure and doped SiS_2 systems with varying doping concentration. (a-d) highest occupied molecular orbitals (HOMO) and (e-h) lowest unoccupied molecular orbitals (LUMO).

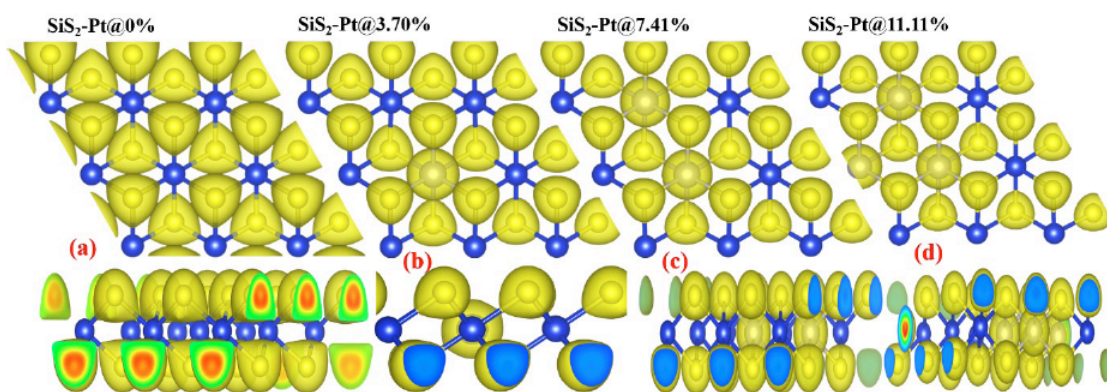


Figure S3: Total electron density in pure and doped SiS₂ monolayers. Isosurface values are set to their default values.

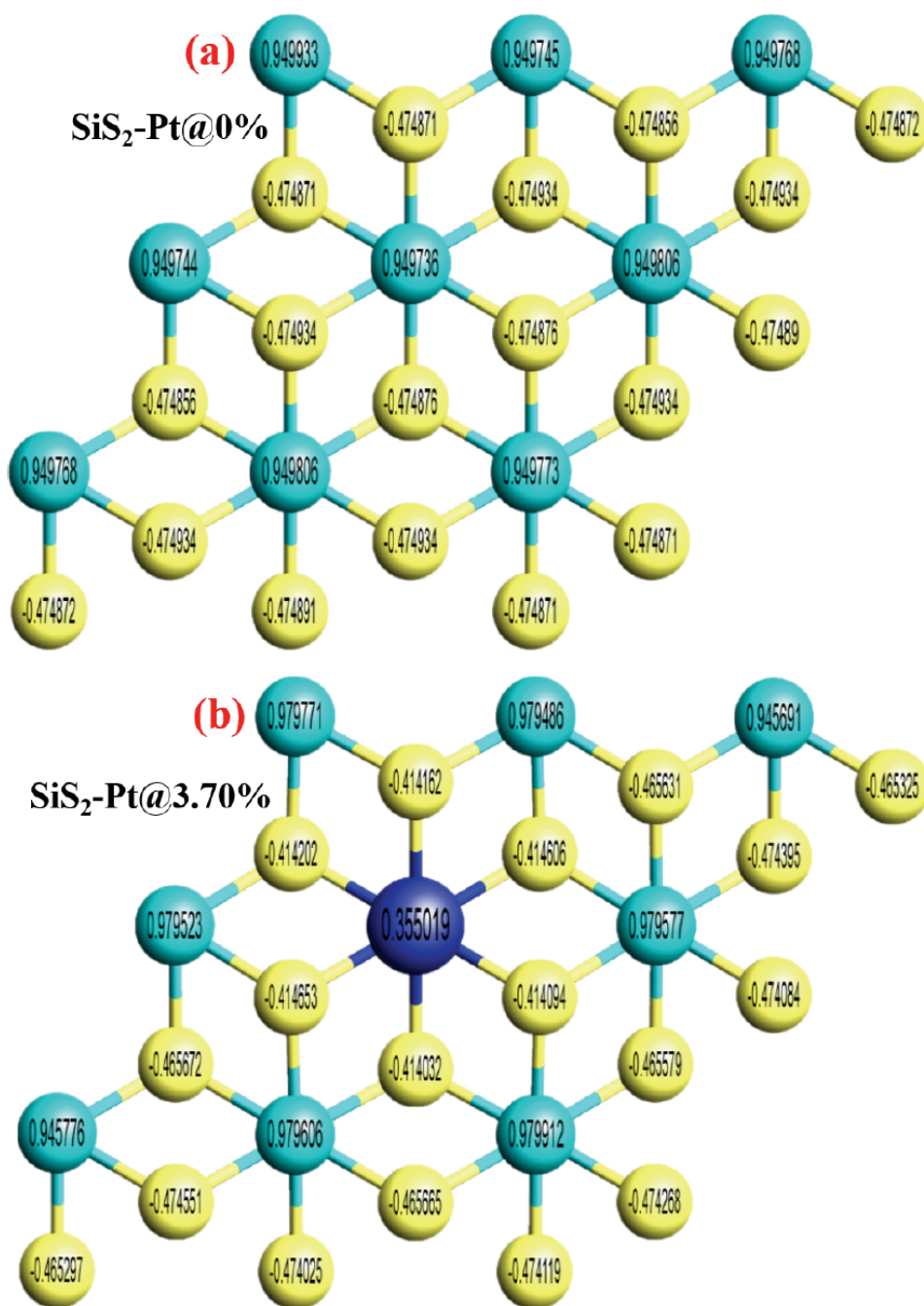


Figure S4: Net charge on each individual constituent atom using the Mulliken population analysis. (a) SiS₂-Pt@0% and (b) SiS₂-Pt@3.70%.

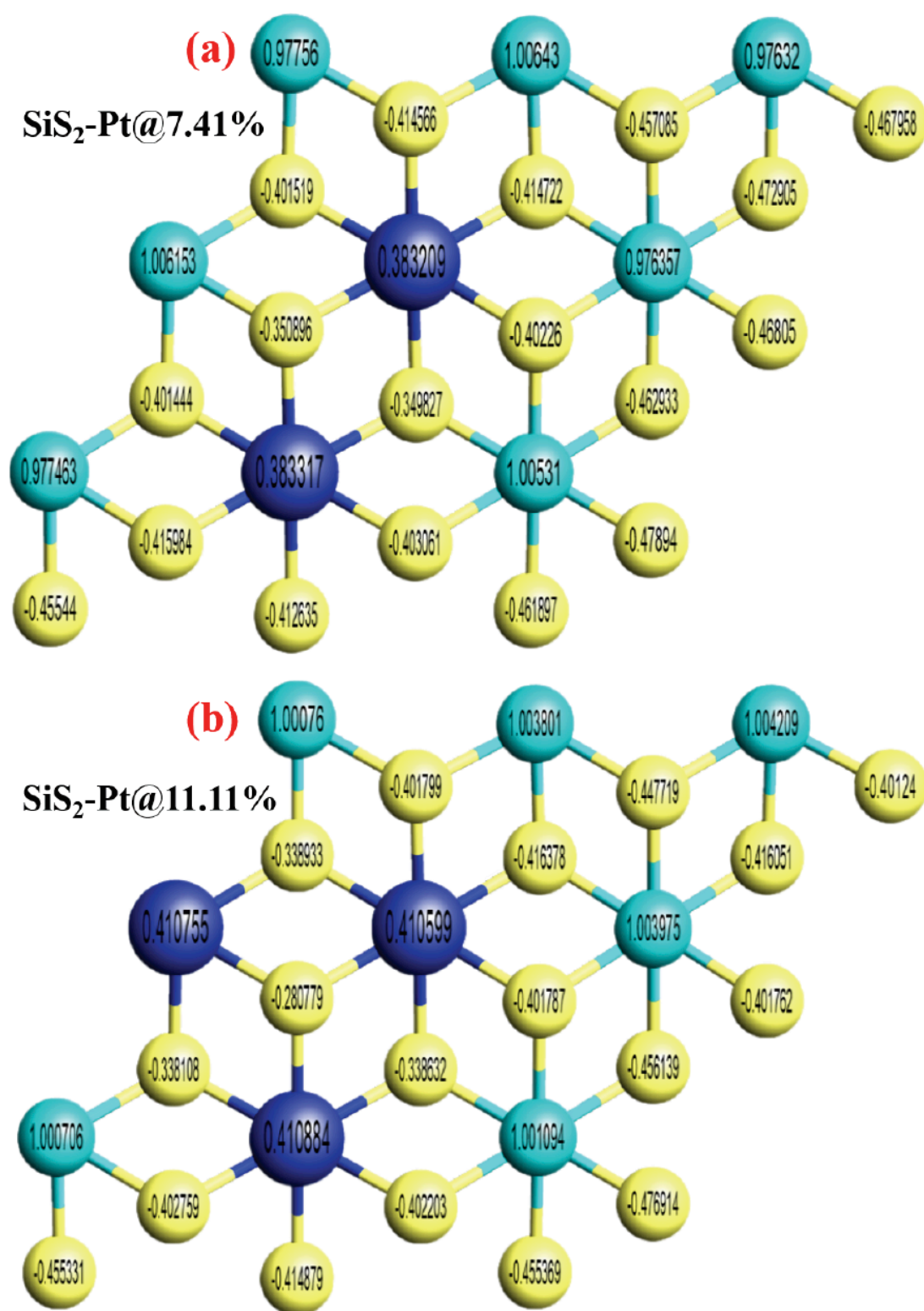


Figure S5: Net charge on each individual constituent atom using the Mulliken population analysis. (a) $\text{SiS}_2\text{-Pt@7.41\%}$ and (b) $\text{SiS}_2\text{-Pt@11.11\%}$.

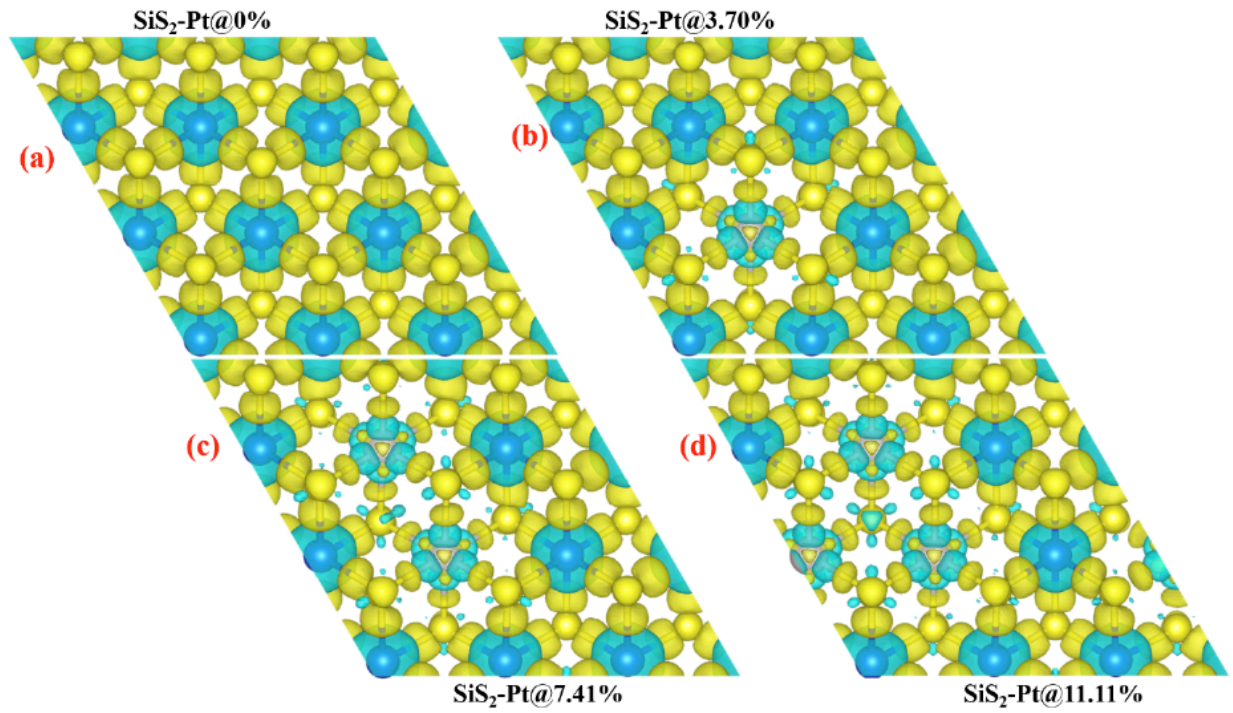


Figure S6: Difference electron densities calculated from atomic densities in pure and doped SiS_2 systems. Isosurface values are set to their default values. The blue color indicates an electron density rich region.

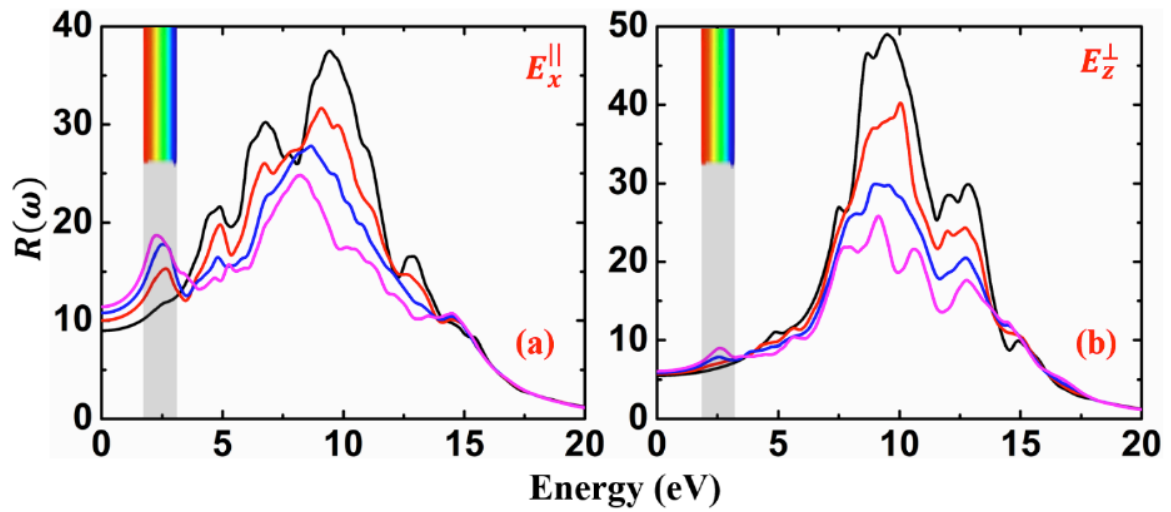


Figure S7: Reflection spectra in pure and doped SiS_2 monolayer materials along (a) x-direction and (b) z-direction, respectively.