Supporting Information

for

Band aliment type I, II transformations in Hf_2CO_2/MoS_2 heterostructures using biaxial strain, external electric field, and interlayer coupling: a first principal investigation

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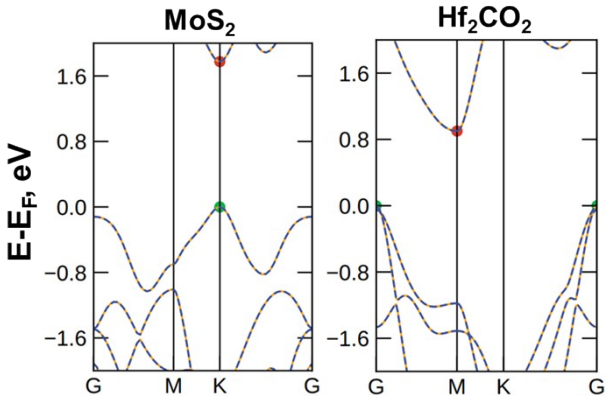

Figure S1. Band structures of pristine separate MoS_2 and Hf_2CO_2 monolayers with respect to Fermi energy value.

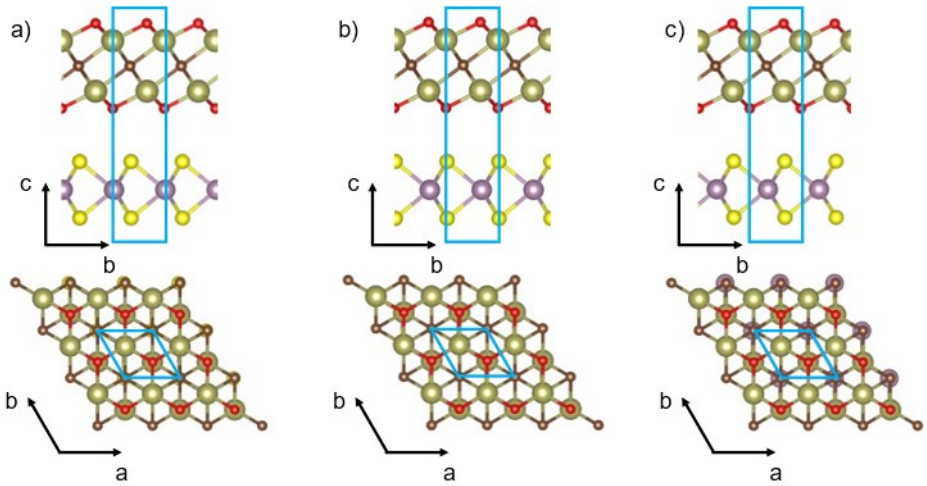

Figure S2. The considered stacking of Hf_2CO_2 and MoS_2 monolayers with the energy calculated relative to the structure in figure c: a) 0.005 eV, b) 0.060 eV, c) 0.000 eV.

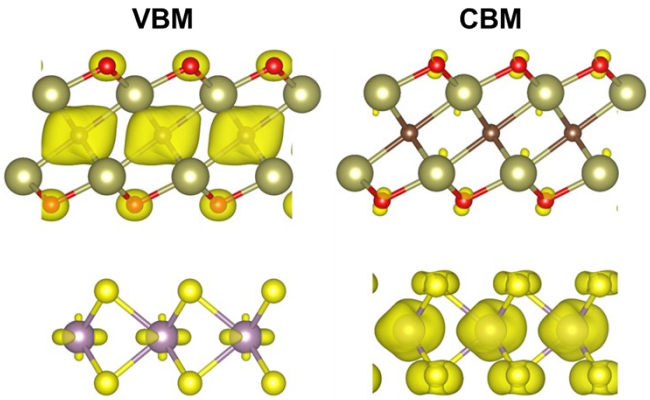

Figure S3. Partial charge density for the band edges of the Hf_2CO_2/MoS_2 heterostructure.

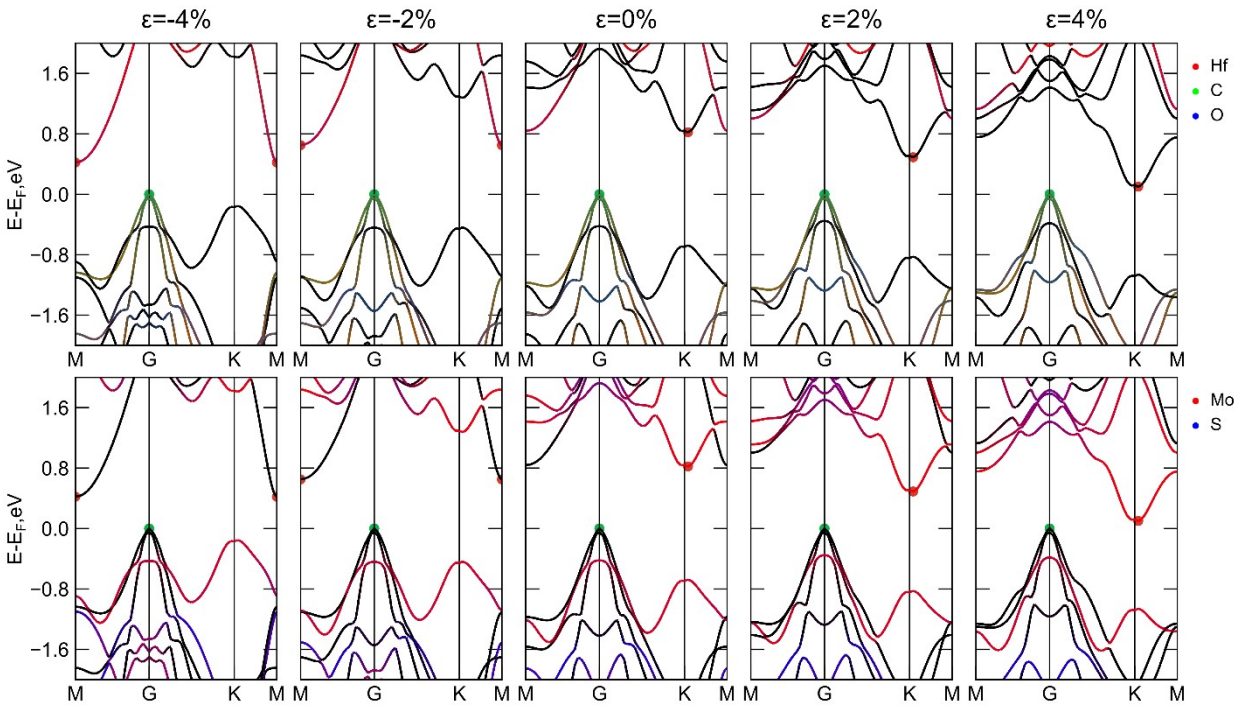

Figure S4. Atom-resolved electronic band structures of biaxially deformed Hf_2CO_2/MoS_2 heterostructure concerning Fermi energy value.

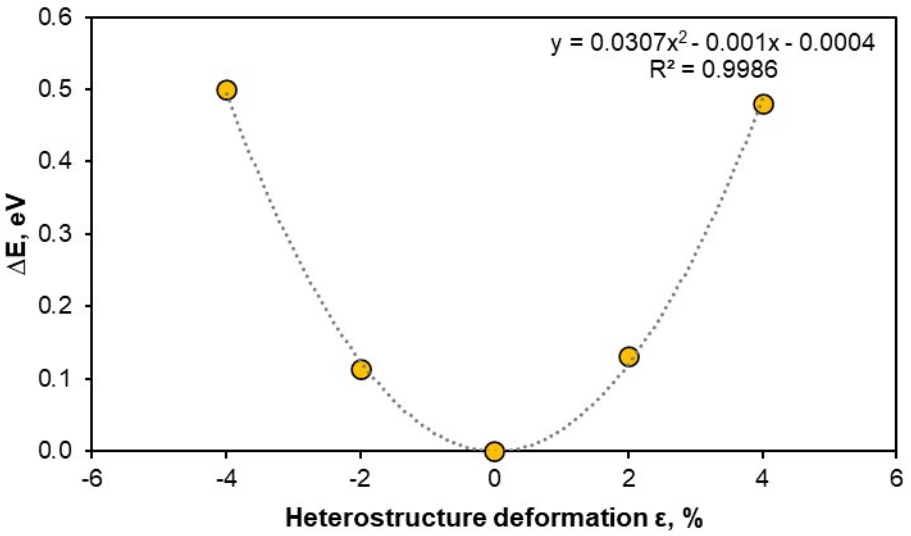

Figure S5. Total energy dependence of biaxially deformed Hf_2CO_2/MoS_2 heterostructure.

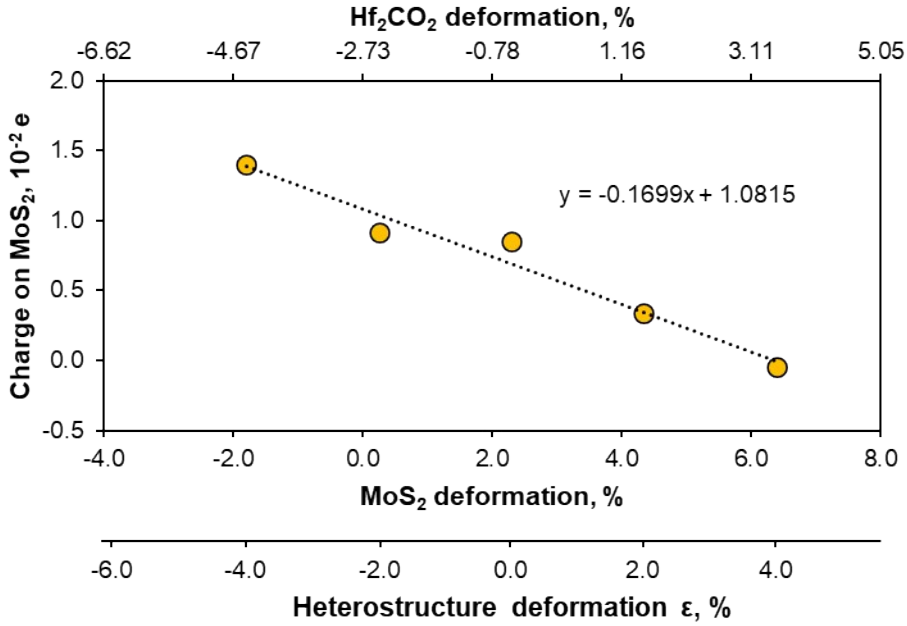

Figure S6. Bader charges analysis of biaxially deformed Hf_2CO_2/MoS_2 heterostructure.

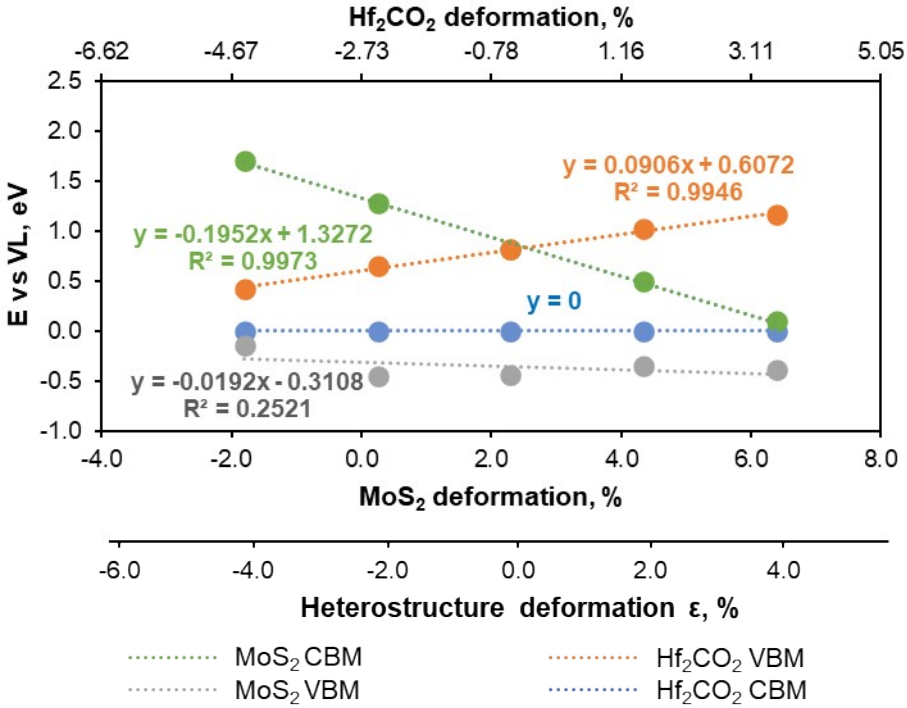

Figure S7. Heterostructure components band edges dependencies on the applied biaxial strain.

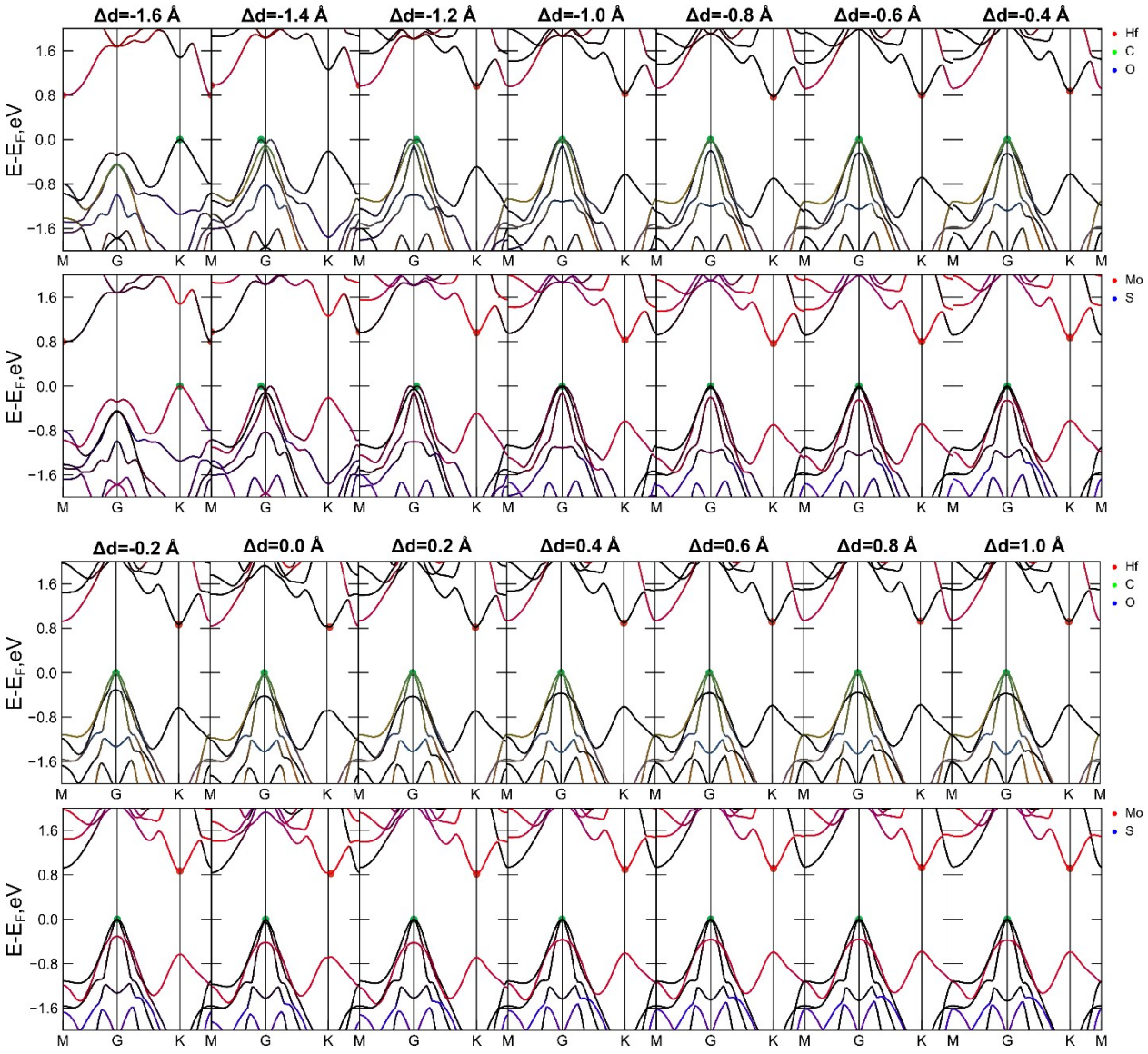

Figure S8. The dependence of the atom-resolved electronic band structures on the interlayer coupling for the Hf_2CO_2/MoS_2 heterostructure concerning Fermi energy value.

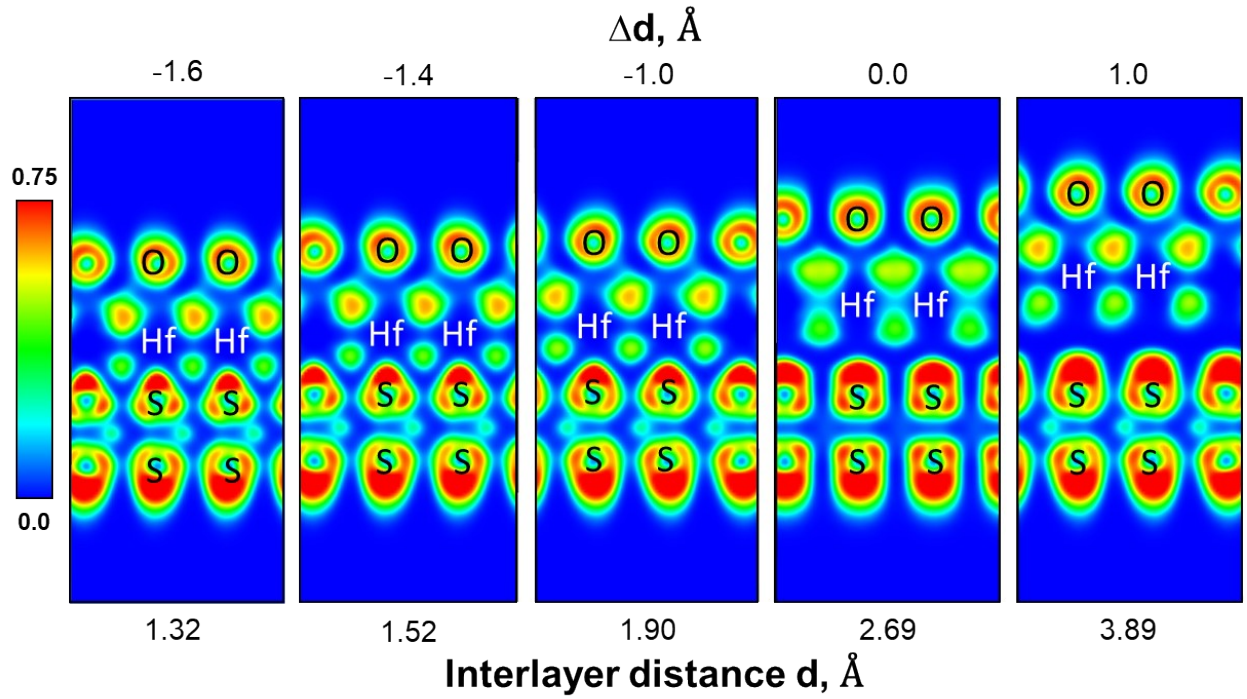

Figure S9. The electron localization function plots the chosen interlayer distances for the Hf_2CO_2/MoS_2 heterostructure.

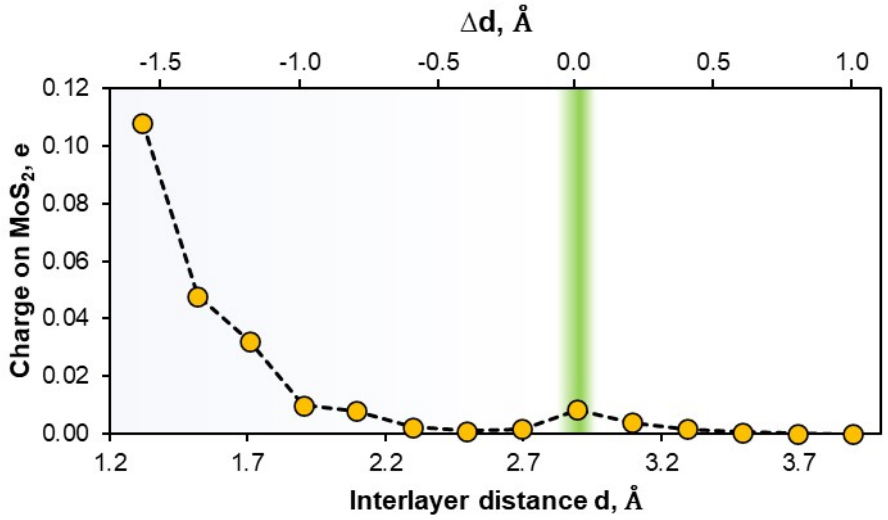

Figure S10. Bader charges analysis for the different interlayer coupled Hf_2CO_2/MoS_2 heterostructures. By the green point, the equilibrium interlayer distance is marked.

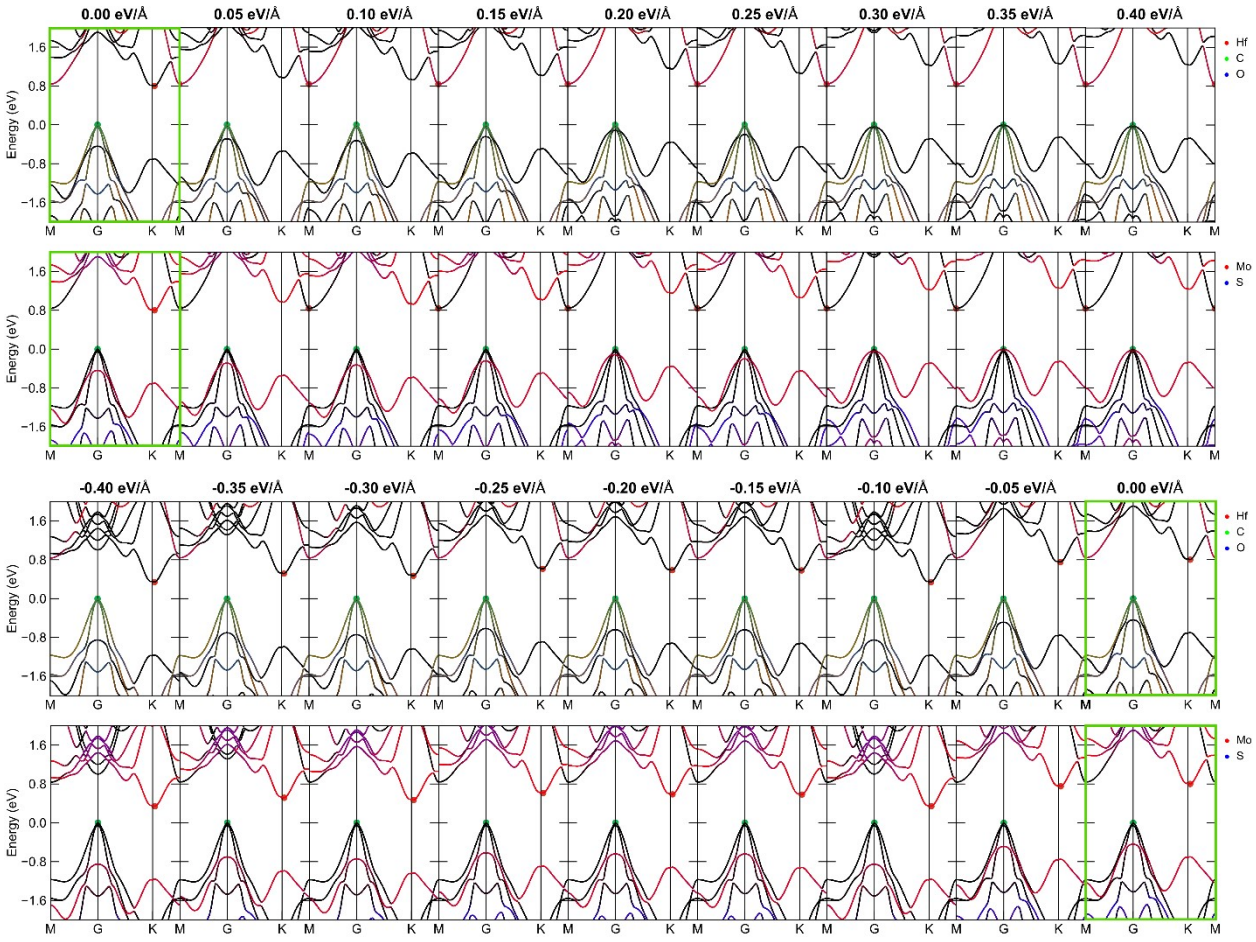

Figure S11. The dependence of the atom-resolved electronic band structures on the applied external electric field for the Hf_2CO_2/MoS_2 heterostructure concerning Fermi energy value. By green frames, the initial band structure is highlighted.

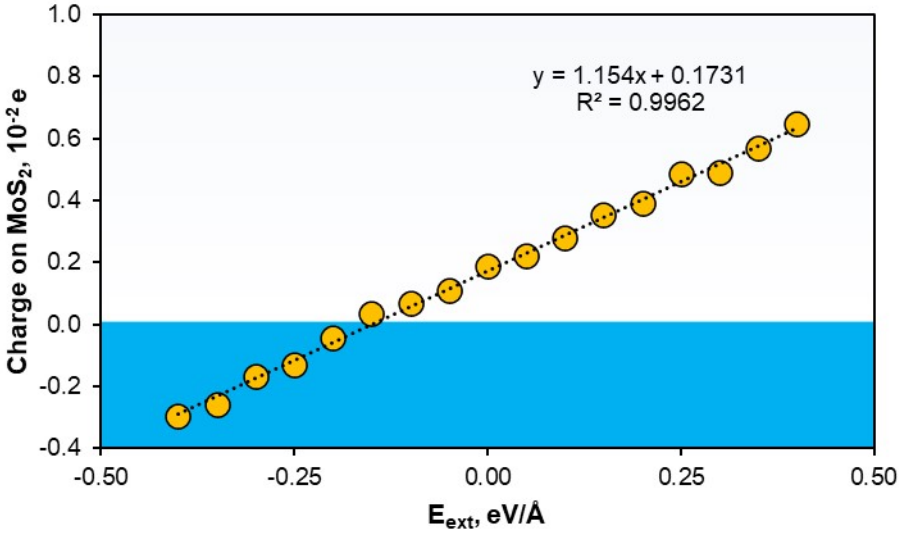

Figure S12. Bader charges analysis for the different values of applied to Hf_2CO_2/MoS_2 heterostructure external electric field.