Supplementary Information

Assessing doping strategies for monolayer MoS_2 towards non-enzymatic detection of cortisol: a first-principles study

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1. Adsorption energies of Ni, Pd, and Pt metals on MoS_2

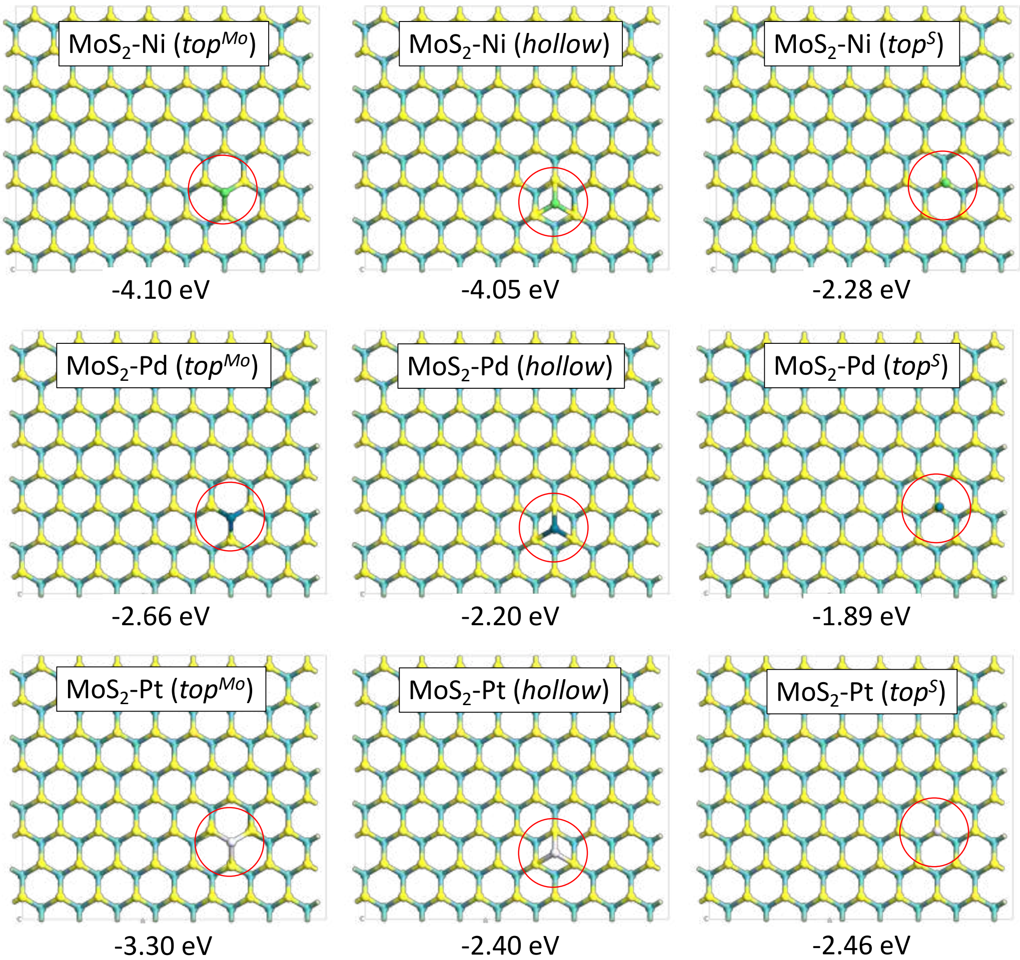

Figure S1. *Adsorption energies of Ni, Pd, and Pt adatoms on* top^{Mo}*, hollow, and* top^{S} *sites of* MoS_2*, computed at the PBE-D2 level.*

2. Bandstructures and HOMO plots of MoS_2/cortisol complexes

Pristine MoS_2

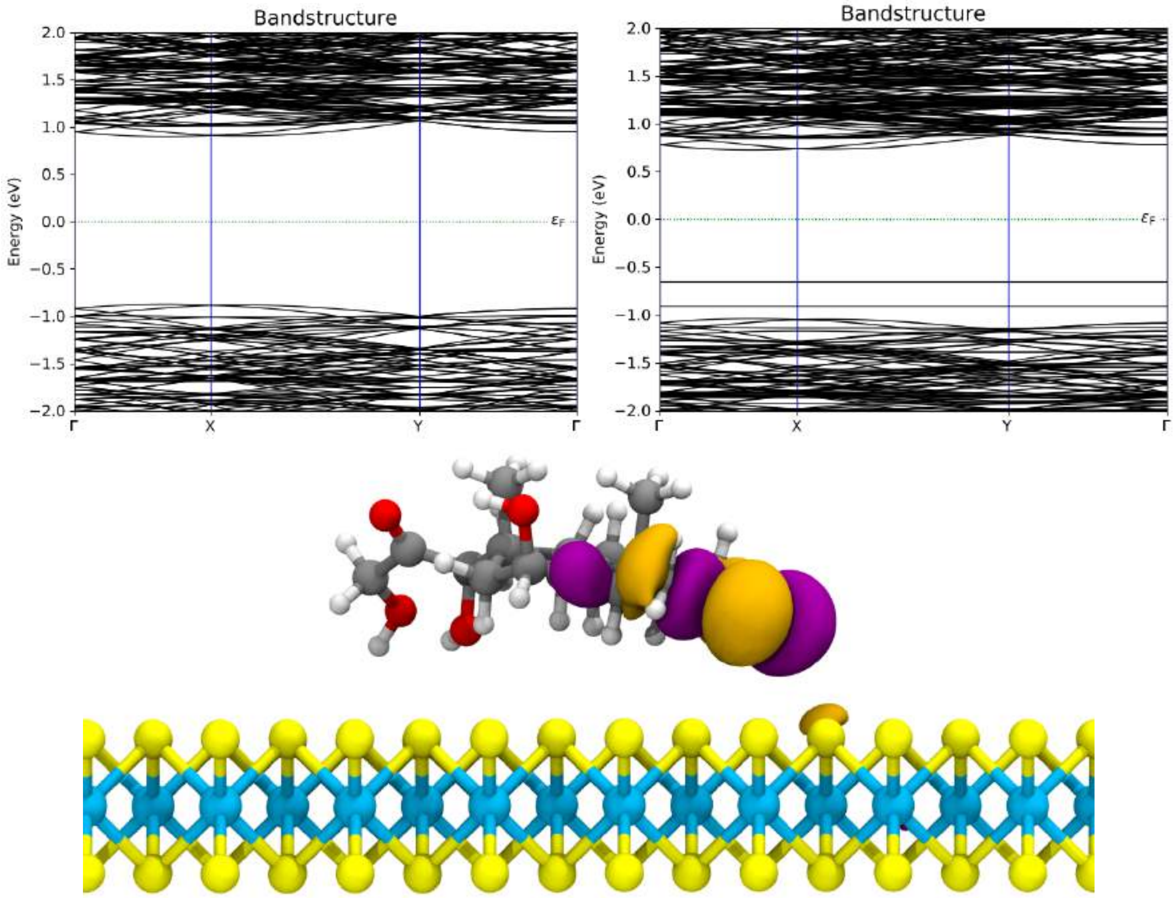

Figure S2. *Computed DFT bandstructure of pristine MoS_2 with (top right) and without (top left) the presence of cortisol. The adsorption of the analyte causes the appearance of extra states above the valence bands of MoS_2, as observed also in the PDOS plot of the complex (see Fig. 8 in the main text). The bottom image shows the HOMO plot of the MoS_2/cortisol system (isovalue 0.02 eV/Å^3).*

Ni-MoS_2

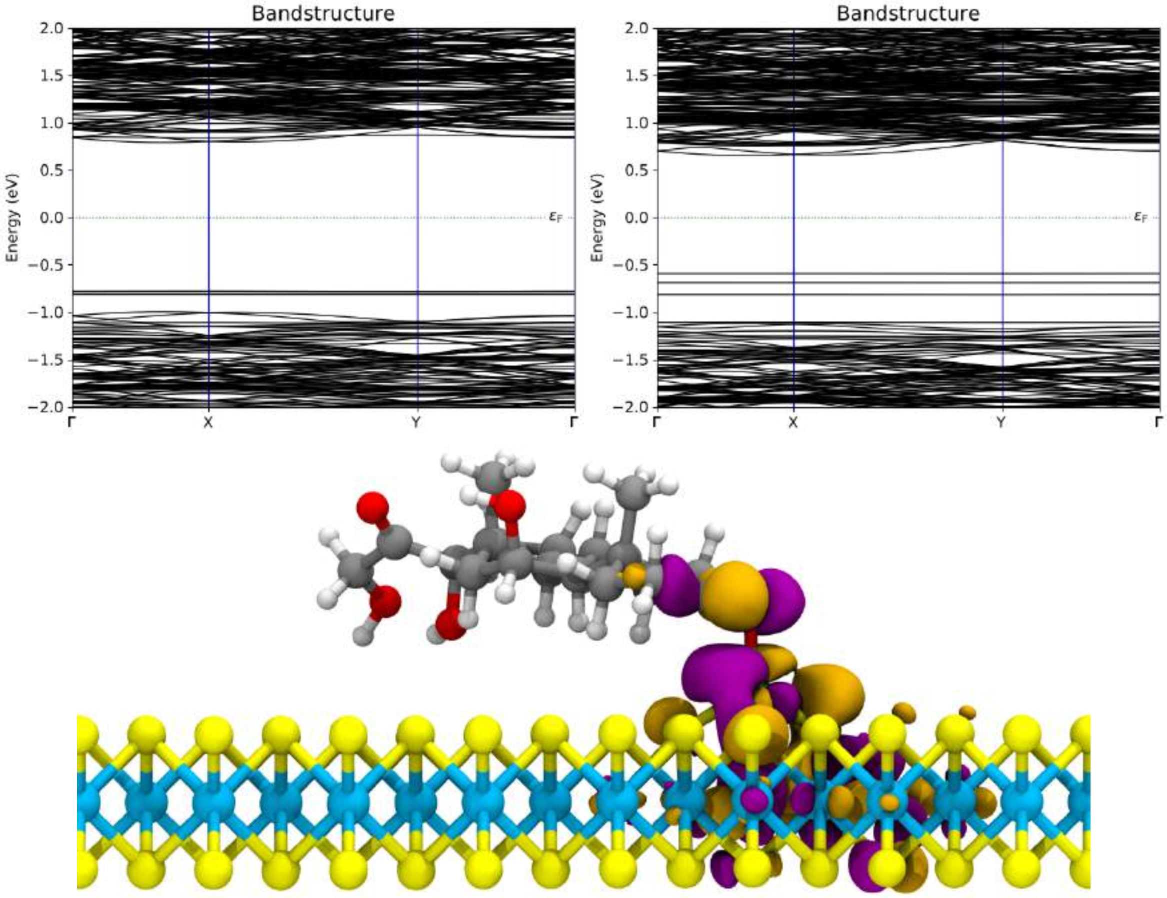

Figure S3. *Computed DFT bandstructure of Ni-MoS_2 with (top right) and without (top left) the presence of cortisol. The adsorption of the analyte causes the broadening of the original bands due to the Ni metal adatom, as well as hybridization between the states of cortisol and those of Ni-MoS_2. This can be observed also in the PDOS plot of the complex (see Fig. 8 in the main text). The bottom image shows the HOMO plot of the Ni-MoS_2/cortisol system (isovalue 0.02 eV/$Å^3$), which further confirms the hybrid nature of the valence bands.*

Pd-MoS_2

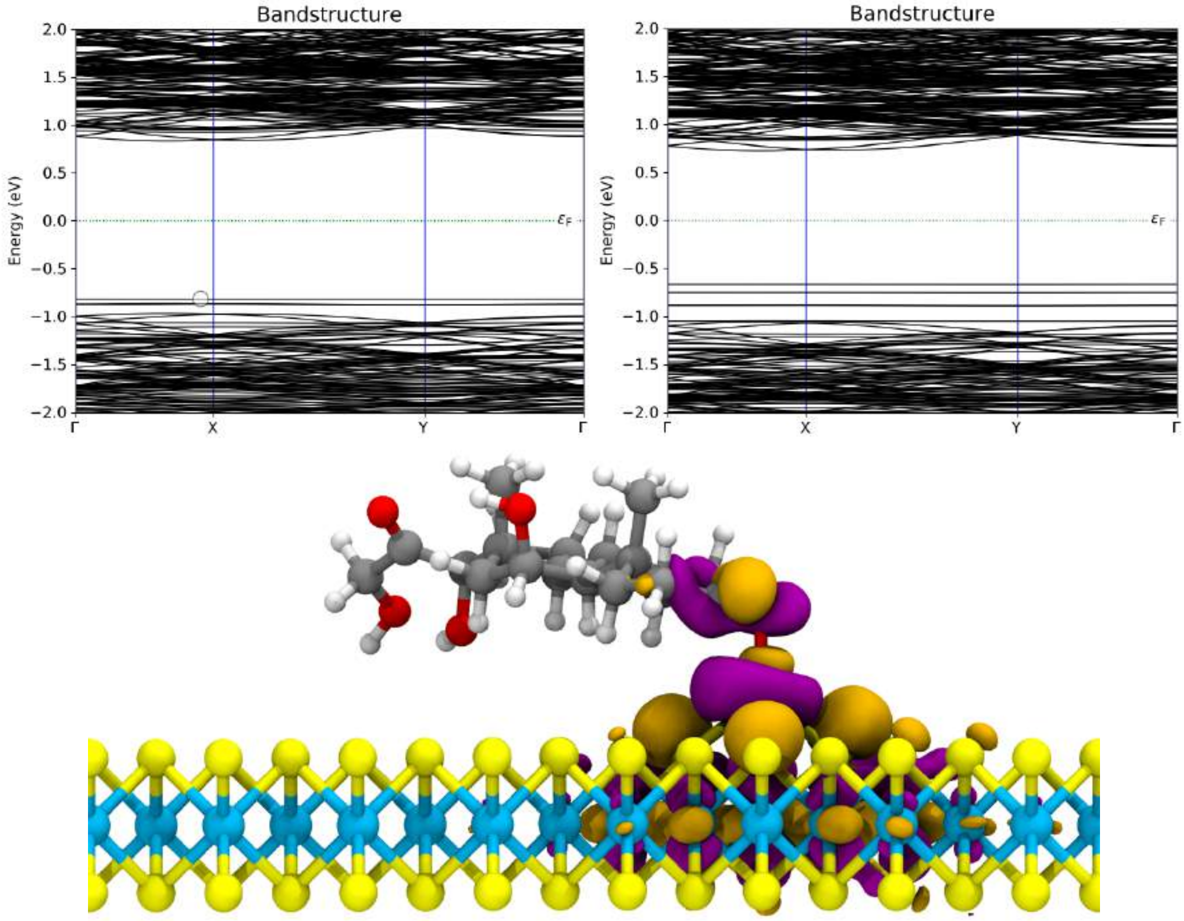

Figure S4. *Computed DFT bandstructure of Pd-MoS_2 with (top right) and without (top left) the presence of cortisol. The adsorption of the analyte causes the broadening of the original bands due to the Pd metal adatom, as well as hybridization between the states of cortisol and those of Pd-MoS_2. This can be observed also in the PDOS plot of the complex (see Fig. 8 in the main text). The bottom image shows the HOMO plot of the Pd-MoS_2/cortisol system (isovalue 0.02 eV/$Å^3$), which further confirms the hybrid nature of the valence bands.*

Pt-MoS_2

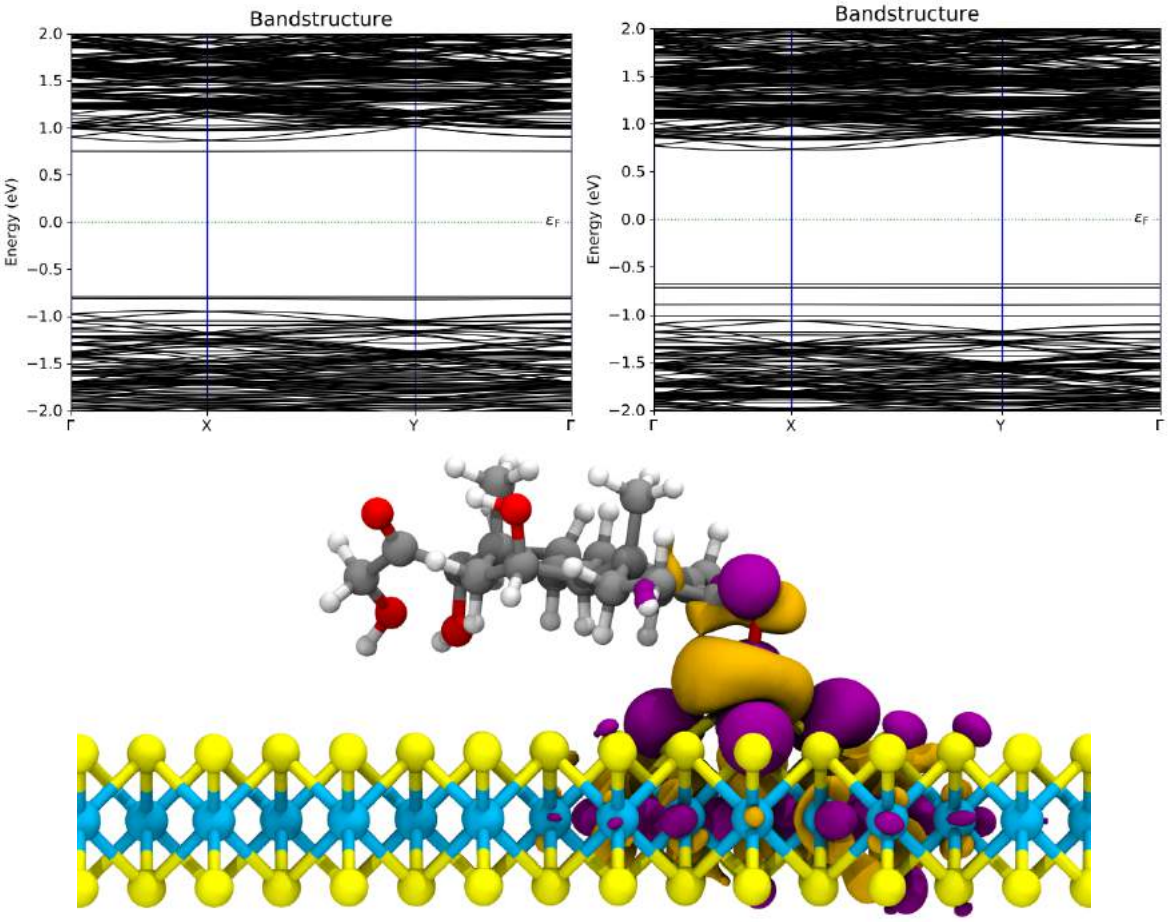

Figure S5. *Computed DFT bandstructure of Pt-MoS_2 with (top right) and without (top left) the presence of cortisol. The adsorption of the analyte causes the broadening of the original bands due to the Pt metal adatom, as well as hybridization between the states of cortisol and those of Pt-MoS_2. The removal of the extra conduction band due to Pt doping upon the analyte adsorption can also be observed. This is consistent with the PDOS plot of the complex (see Fig. 8 in the main text). The bottom image shows the HOMO plot of the Pt-MoS_2/cortisol system (isovalue 0.02 eV/Å^3), which further confirms the hybrid nature of the valence bands.*