Supplementary Information for "Theoretical prediction of structural characteristics and SO_2 adsorption-sensing properties of the pristine HfS_2 and TM-doped HfS_2 monolayers (TM = Ni, Pd, or Pt)"

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TABLE S1: The convergence test of the total energy of the 3 × 3 - dimensional HfS_2 supercell in the K-points grid dependence. The calculated total energy using the k-points grid of 5 x 5 x 1 and the cutoff energy of 500 eV reaches the convergence of 10^{-4} eV, indicating that these parameters are sufficient to obtain reliable results.

Kpoint grid	Total energy (eV)
3 x 3 x 1	-209.57658
4 x 4 x 1	-209.58383
5 x 5 x 1	-209.58354
6 x 6 x 1	-209.58357
7 x 7 x 1	-209.58356
8 x 8 x 1	-209.58358

TABLE S2: The calculated total energies and the currents flowing through the sensor device based on the Pt-doped HfS_2 monolayer at the bias voltage of 10 mV using the TRANSIESTA code in dependence on the K-points grid. The cutoff enerrgy was set to 300 Ry.

K-point grid	Total energy (eV)	Current (μA)
20 x 1 x 1	-152436.8689	1.4105
40 x 1 x 1	-152436.8703	1.4102
60 x 1 x 1	-152436.8639	1.4103
80 x 1 x 1	-152436.8643	1.4102
100 x 1 x 1	-152436.8637	1.4103

TABLE S3: The calculated total energies and the currents flowing through the sensor device based on the Pt-doped HfS_2 monolayer at the bias voltage of 10 mV using the TRANSIESTA code in dependence on the cutoff energy. K-points grid was set to 300 Ry. The calculated currents using the k-points grid of 100 x 1 x 1 and the cutoff energy of 300 Ry reaches the convergence of approximately 10^{-4} eV, indicating that these parameters are sufficient to obtain reliable results in the TRANSIESTA calculations.

Cutoff energy (Ry)	Total energy (eV)	Current (μA)
100	-152437.5841	1.4128
150	-152437.1072	1.4109
200	-152436.9428	1.4115
250	-152436.9106	1.4107
300	-152436.8637	1.4103
350	-152436.8488	1.4105

TABLE S4: The calculated total energies of the TM-doped HfS_2 monolayer (TM=Ni, Pd, or Pt). The smallest values in bold indicate total energies of the most stable configurations for Ni-, Pd- and Pt-doping on the HfS_2 monolayer. The position symbols (A, B, C) are explained on Figure S2.

TM-adatom	Positions	The total energies (eV)
Ni	A	-211.9433
	B	-214.1521
	C	**-214.7490**
Pd	A	-212.8092
	B	-213.9851
	C	**-214.3944**
Pt	A	-212.4810
	B	-214.1271
	C	**-214.7131**

TABLE S5: The calculated adsorption energies of SO_2 monolecule on the TM-doped HfS_2 monolayer (TM=Ni, Pd, Pt). The smallest values in bold indicate adsoprtion energies of the most stable adsorption configurations of SO_2 molecule on the Ni-, Pd- and Pt-doped HfS_2 monolayer, respectively. H, V $_1$, and V $_2$ show the initial orientation of the SO_2 molecule in structural optimizations, which corresponds to horizontal orientation and vertical orientations, with atom S below and atom S above.

Orientations	The adsorption energies on TM-doped HfS_2 monolayer (eV)		
	Ni-doped	Pd-doped	Pt-doped
H	-0.845	-0.753	-0.825
V_1	**-0.847**	**-0.758**	**-0.826**
V_2	-0.426	-0.501	-0.459

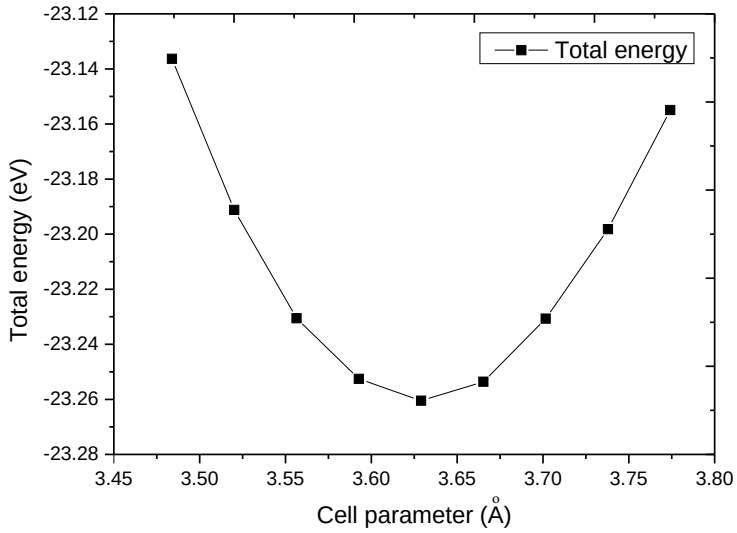

FIG. S1: The dependence of the total energy of the relaxed unit-cell HfS_2 monolayer on the assumed cell parameter. The lowest total energy achieves at a = 3.63 Å, indicating this value is the optimized cell parameter of the HfS_2 monolayer.

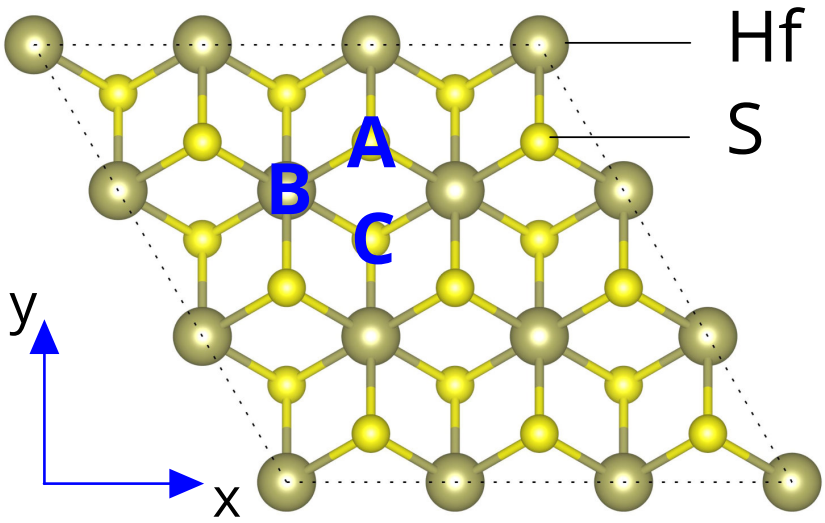

FIG. S2: Doping positions of TM-atoms on the HfS_2 monolayer (TM= Ni, Pd, or Pt). A, B and C are the upper position of the S atom in the top layer, the upper position of the Hf atom and the hollow position, respectively.