Table 1 - DFT results of the Bi_2S_3 and MoS_2 supercells with added H_20 molecules.

		Number of added H_20 Molecules				
		0	1	2	3	4
Bi_2S_3 Supercell (88,21 Å^2)	S-S Distance (Å)	1.68	0.83	1.43	2.66	3.03
	$E_{D\text{-}Bi2S3}$ (eV)	-185.87	-199.87	-214.34	-228.34	-243.17
	$E_{2D\text{-}Bi2S3}$ (eV)	-182.46	-196.92	-210.99	-225.67	-240.26
	$\Delta E_{sep\text{-}Bi2S3}$/Area (eV/Å^2)[a]	0.038	0.033	0.038	0.030	0.033
MoS_2 Supercell (69,58 Å^2)	S-S Distance (Å)	3.02	4.49	5.29	5.77	5.95
	$E_{D\text{-}MoS2}$ (eV)	-362.12	-375.86	-390.47	-405.15	-419.98
	$E_{2D\text{-}MoS2}$ (eV)	-360.30	-375.22	-389.52	-404.10	-418.43
	$\Delta E_{sep\text{-}MoS2}$/Area (eV/Å^2)[a]	0.026	0.009	0.014	0.015	0.022

[a] Energy difference between the two sulfide layers and the two layers plus H_20 molecules, per unit area (surface energy).

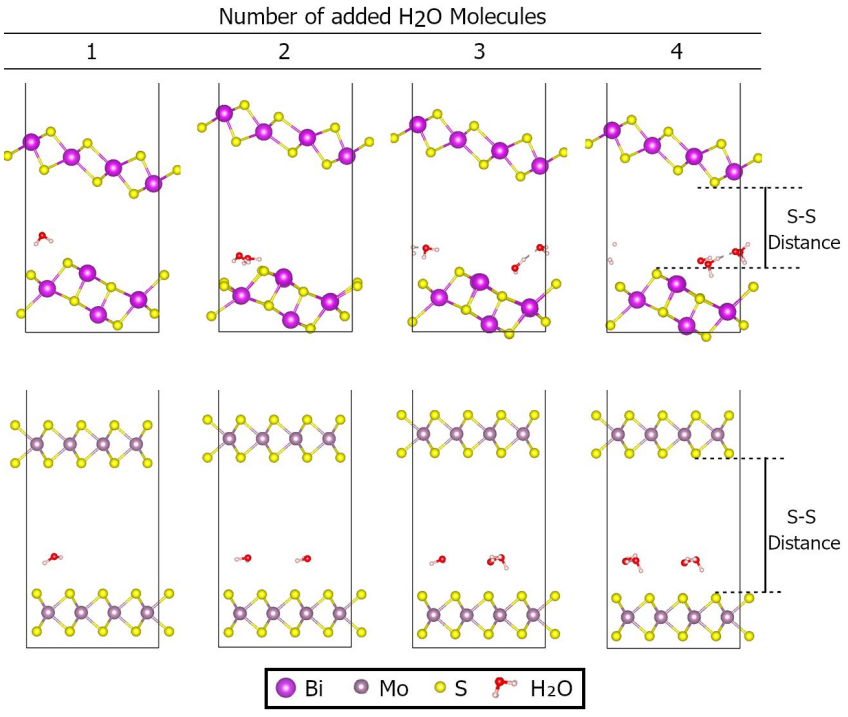

Fig. 1 – DFT modeling of the sulfide supercells (2D) with added H_20 molecules.