

Supplementary Information

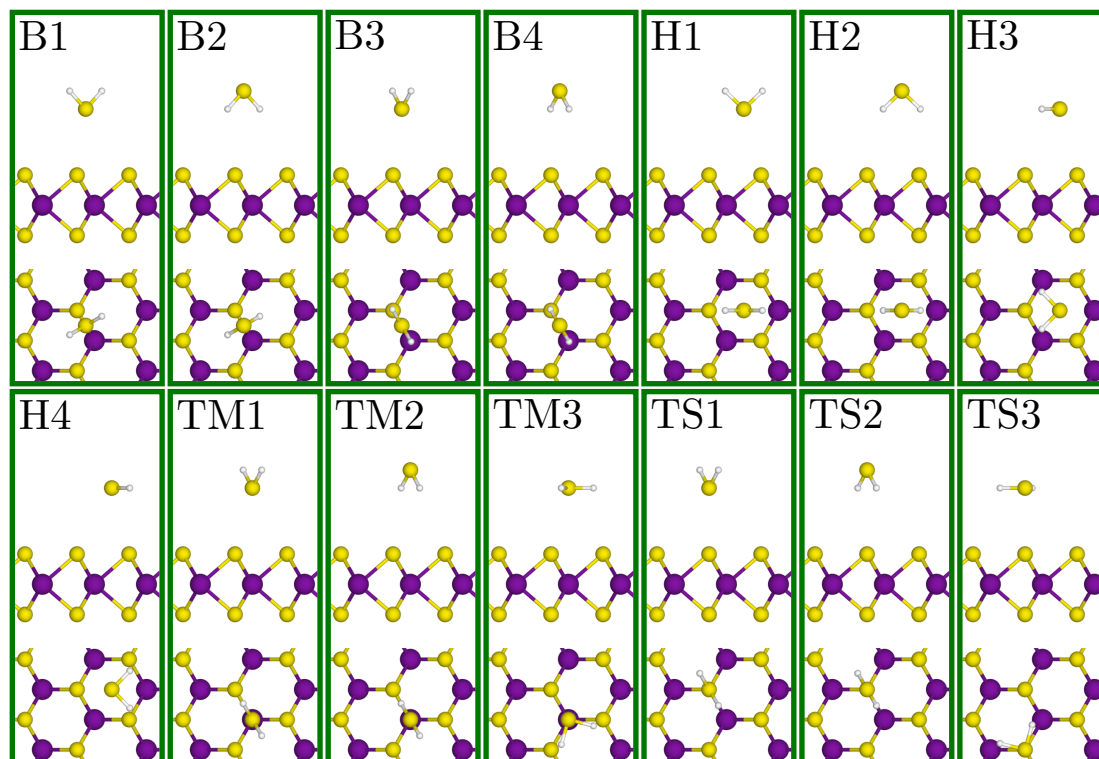


Fig. S1 Initial configurations for the adsorption of H₂S molecule above the SL-MoS₂ surface. Purple (yellow) atoms represent Molybdenum (Sulfur).

Table S1 Zero-crossing energies for the real part of the dielectric function spectra (ϵ_1) for pristine and H₂S adsorbed SL-MoS₂ under different strains and concentrations of gas molecules.

System	Strain (%)	Num. of H ₂ S Mol.	1st	2nd	3rd	4th	5th	6th	7th	8th	9th	10th
SL-MoS ₂	-8	None	4.641	6.591	7.384	8.321	12.33	13.11	15.32	-	-	-
		1	4.608	6.555	7.361	12.34	13.18	15.36	16.36	-	-	-
		2	4.585	6.524	7.342	12.36	13.26	15.4	16.41	-	-	-
		3	4.565	6.489	7.323	12.39	13.3	15.48	16.5	-	-	-
		4	4.525	6.34	7.325	12.37	13.41	15.54	16.49	-	-	-
	-6	None	4.657	7.298	7.59	8.181	12.99	13.73	15.11	15.98	-	-
		1	4.642	6.493	7.274	8.08	13.01	13.71	15.17	16.03	-	-
		2	4.629	6.45	7.248	13.06	15.24	16.13	-	-	-	-
		3	4.622	6.409	7.212	13.09	16.35	-	-	-	-	-
		4	4.539	6.292	7.229	8.112	12.22	13.1	16.34	-	-	-
	-4	None	4.693	7.238	8.059	12.83	13.74	14.44	14.94	15.56	-	-
		1	4.682	7.216	7.987	12.85	13.75	14.53	14.99	15.68	-	-
		2	4.664	7.193	7.849	12.87	13.76	16.02	-	-	-	-
		3	4.645	7.167	12.91	16.11	-	-	-	-	-	-
		4	4.605	6.193	7.177	8.12	12.93	16.11	-	-	-	-
	-2	None	4.665	7.138	8.276	13.72	14.4	14.83	15.47	-	-	-
		1	4.652	7.127	7.821	8.238	13.76	14.47	14.86	15.55	-	-
		2	4.643	7.114	7.696	8.194	14.53	14.9	15.68	-	-	-
		3	4.629	7.101	7.542	7.565	7.581	15.79	-	-	-	-
		4	4.586	6.093	7.109	7.507	8.24	15.87	-	-	-	-
	0	None	3.06	4.516	5.438	7.058	7.542	8.07	14.15	15.45	-	-
		1	3.009	4.517	5.434	7.037	7.469	7.991	14.33	15.37	-	-
		2	2.984	4.519	5.43	7.016	7.937	14.38	15.28	-	-	-
		3	2.969	4.522	5.425	6.986	7.897	11.98	14.42	15.2	-	-
		4	2.968	4.476	5.403	5.796	7.05	7.447	7.921	11.9	14.49	15.36
	2	None	3.005	5.372	6.97	7.966	13.99	15.23	-	-	-	-
		1	2.988	5.366	6.82	6.927	7.738	13.99	15.2	-	-	-
		2	2.971	5.36	6.787	7.681	14	15.17	-	-	-	-
		3	2.954	5.353	6.76	7.647	11.99	14	15.13	-	-	-
		4	2.941	5.339	6.74	6.96	7.682	11.9	14.08	14.39	15.2	-
	4	None	2.84	5.313	5.815	6.732	7.718	13.84	-	-	-	-
		1	2.839	5.309	5.816	6.69	7.687	13.84	-	-	-	-
		2	2.835	5.305	5.816	6.655	7.662	13.86	-	-	-	-
		3	2.826	5.299	5.815	6.629	7.638	11.98	13.87	-	-	-
		4	2.808	5.29	5.803	6.67	7.683	13.96	14.73	-	-	-
	6	None	2.685	5.152	5.559	6.539	7.508	13.65	-	-	-	-
		1	2.689,	5.16	5.558	6.508	7.464	13.64	-	-	-	-
		2	2.693,	5.554	6.477	7.427	13.62	-	-	-	-	-
		3	2.697,	5.548	6.453	7.393	11.97	13.58	-	-	-	-
		4	2.693,	5.537	7.368	-	-	-	-	-	-	-
8	None	2.526,	5.366	7.237	14.11	-	-	-	-	-	-	
	1	2.532	5.364	7.212	-	-	-	-	-	-	-	
	2	2.539	5.362	7.192	-	-	-	-	-	-	-	
	3	2.546	5.358	7.176	-	-	-	-	-	-	-	
	4	2.549	5.351	7.159	-	-	-	-	-	-	-	

Table S2 Energies and (relative) intensities of the first ten peaks in the EEL spectra for different strains and concentrations of H₂S molecules introduced to SL-MoS₂ sheet.

System	Strain (%)	Num. of H ₂ S Mol.	1st	2nd	3rd	4th	5th	6th	7th	8th	9th	10th	
-8		None	(16.94,2.514)	(16.41,2.404)	(16.57,2.237)	(15.35,2.096)	(17.92,1.897)	(18.5,1.834)	(18.8,1.824)	(18.16,1.768)	(15.79,1.483)	(17.35,1.441)	
		1	(16.94,2.571)	(16.42,2.35)	(16.6,2.288)	(17.94,2.012)	(15.36,1.998)	(18.5,1.914)	(18.8,1.895)	(18.76,1.89)	(18.76,1.89)	(18.66,1.867)	(18.33,1.729)
		2	(16.96,2.611)	(16.63,2.351)	(16.44,2.29)	(17.96,2.138)	(18.52,2.003)	(18.72,1.983)	(18.76,1.979)	(18.68,1.978)	(18.68,1.978)	(18.62,1.967)	(15.37,1.892)
		3	(17.02,2.653)	(16.64,2.394)	(17.96,2.24)	(18.52,2.123)	(18.64,2.086)	(18.68,2.086)	(18.33,1.91)	(17.53,1.826)	(17.53,1.826)	(15.39,1.776)	(20.36,1.425)
-6		None	(17.2,5.38)	(16.66,2.321)	(17.96,2.268)	(18.52,2.201)	(18.7,2.161)	(18.66,2.158)	(18.74,2.158)	(17.51,1.874)	(15.4,1.694)	(20.36,1.489)	
		1	(16.76,2.392)	(16.36,2.382)	(16.09,2.061)	(17.58,1.854)	(18.58,1.831)	(18.54,1.827)	(17.94,1.817)	(17.94,1.817)	(15.16,1.675)	(15.62,1.6)	(18.17,1.583)
		2	(16.78,2.436)	(16.37,2.39)	(17.6,1.952)	(18.58,1.929)	(18.54,1.921)	(17.92,1.905)	(18.17,1.667)	(18.17,1.667)	(15.17,1.621)	(15.64,1.554)	(17.15,1.522)
		3	(16.8,2.473)	(16.39,2.38)	(17.6,2.065)	(18.58,2.018)	(18.54,2.011)	(17.92,2.007)	(18.17,1.763)	(18.17,1.763)	(17.17,1.661)	(15.18,1.556)	(15.64,1.502)
-4		None	(16.8,2.511)	(16.45,2.355)	(17.6,2.17)	(17.92,2.102)	(18.56,2.081)	(18.6,2.078)	(18.52,2.077)	(18.48,2.071)	(18.15,1.874)	(17.17,1.789)	
		1	(16.82,2.443)	(16.56,2.293)	(17.68,2.216)	(17.94,2.183)	(18.56,2.182)	(18.6,2.177)	(18.52,2.174)	(18.15,1.972)	(17.17,1.754)	(15.23,1.421)	
		2	(16.1,2.364)	(16.56,2.113)	(18.3,1.972)	(15.68,1.836)	(17.42,1.803)	(17.04,1.795)	(17.7,1.702)	(17.7,1.702)	(17.19,1.698)	(16.81,1.624)	(8.62,1.575)
		3	(16.16,2.342)	(16.56,2.133)	(18.3,2.057)	(17.04,1.905)	(17.4,1.9)	(15.73,1.807)	(16.81,1.714)	(17.93,1.55)	(14.99,1.406)	(8.6,1.317)	
0		None	(16.22,2.332)	(16.56,2.169)	(18.32,2.127)	(17.4,2.023)	(17.04,1.994)	(16.81,1.808)	(17.93,1.643)	(15.1,354)	(19.82,1.284)	(19.21,1.235)	
		1	(16.26,2.313)	(16.58,2.216)	(18.34,2.193)	(17.42,2.129)	(17.04,2.071)	(17.93,1.735)	(19.82,1.351)	(19.56,1.296)	(15,1,295)	(19.25,1.293)	
		2	(18.32,2.287)	(16.27,2.248)	(17.5,2.195)	(17.46,2.194)	(17.54,2.193)	(16.58,2.144)	(17.08,2.006)	(17.95,1.821)	(19.84,1.395)	(19.56,1.376)	
		3	(15.96,2.358)	(18.1,2.058)	(18.14,2.053)	(18.06,2.051)	(8.28,1.948)	(16.92,1.945)	(17.5,1.647)	(16.27,1.605)	(17.67,1.458)	(17.33,1.421)	
-2		None	(16.2,31)	(18.08,2.133)	(18.12,2.124)	(18.04,2.123)	(16.94,2.036)	(8.27,1.731)	(16.35,1.693)	(17.5,1.655)	(17.35,1.589)	(17.67,1.536)	
		1	(16.03,2.281)	(18.08,2.198)	(18.12,2.193)	(18.04,2.186)	(16.96,2.118)	(16.84,2.085)	(16.82,2.083)	(17.41,1.716)	(17.45,1.715)	(17.67,1.606)	
		2	(18.08,2.251)	(18.12,2.247)	(16.06,2.245)	(18.04,2.243)	(18.16,2.237)	(16.96,2.213)	(16.82,2.157)	(17.16,2.11)	(17.69,1.668)	(8.26,1.428)	
		3	(18.16,2.33)	(18.12,2.319)	(16.04,2.225)	(17.22,2.159)	(16.82,2.128)	(17.69,1.773)	(8.28,1.508)	(16.63,1.451)	(19.3,1.394)	(19.01,1.303)	
SL-MoS ₂		None	(15.52,2.234)	(15.64,2.17)	(16.7,2.169)	(17.8,2.141)	(8.3,2.011)	(16.32,1.839)	(8.09,1.823)	(16.03,1.518)	(17.31,1.409)	(17.39,1.398)	
		1	(16.7,2.252)	(17.82,2.198)	(15.51,1.926)	(16.34,1.921)	(15.8,1.877)	(7.99,1.719)	(8.28,1.618)	(17.03,1.526)	(17.07,1.525)	(17.31,1.481)	
		2	(16.74,2.32)	(17.82,2.258)	(16.38,1.995)	(15.9,1.903)	(17.1,1.706)	(17.03,1.694)	(15.5,1.671)	(7.93,1.667)	(17.39,1.546)	(8.24,1.35)	
		3	(16.76,2.383)	(17.84,2.309)	(17.1,1.903)	(16.08,1.804)	(17.43,1.637)	(7.9,1.614)	(15.27,1.48)	(19.34,1.36)	(19.02,1.352)	(18.67,1.26)	
2		None	(16.7,2.252)	(17.8,2.198)	(15.51,1.926)	(16.34,1.921)	(15.8,1.877)	(7.99,1.719)	(8.28,1.618)	(17.03,1.526)	(17.07,1.525)	(17.31,1.481)	
		1	(8.02,2.276)	(16.46,2.263)	(15.3,2.085)	(17.52,1.976)	(17.62,1.936)	(17.66,1.929)	(16.04,1.739)	(7.69,1.619)	(14.01,1.28)	(14.61,1.241)	
		2	(16.48,2.371)	(17.6,2.017)	(17.64,2.014)	(17.56,2.012)	(17.68,2.003)	(8.1,983)	(15.28,1.911)	(16.06,1.797)	(7.67,1.644)	(16.85,1.355)	
		3	(16.5,2.421)	(17.68,2.09)	(17.64,2.084)	(15.26,1.772)	(7.98,1.73)	(7.64,1.658)	(16.93,1.486)	(16.85,1.485)	(16.89,1.483)	(17.07,1.466)	
4		None	(16.54,2.458)	(17.72,2.151)	(7.63,1.666)	(15.24,1.644)	(16.93,1.642)	(16.87,1.642)	(17.09,1.609)	(7.96,1.515)	(18.78,1.375)	(19.02,1.333)	
		1	(16.54,2.403)	(17.7,2.06)	(17.74,2.056)	(18.14,1.866)	(18.1,1.862)	(15.28,1.676)	(16.87,1.639)	(16.93,1.638)	(17.05,1.617)	(7.98,1.604)	
		2	(7.74,3.113)	(16.24,2.264)	(17.42,1.904)	(17.62,1.784)	(17.58,1.78)	(15.42,1.746)	(15.86,1.727)	(17.98,1.282)	(14.63,1.238)	(18.72,1.22)	
		3	(7.71,2.842)	(16.28,2.333)	(17.46,1.925)	(17.42,1.917)	(17.6,1.863)	(17.64,1.858)	(15.4,1.609)	(15.18,1.571)	(17.98,1.351)	(18.72,1.26)	
6		None	(7.69,2.597)	(16.32,2.393)	(17.5,1.98)	(17.46,1.972)	(17.6,1.95)	(17.64,1.943)	(15.1,1.524)	(15.38,1.505)	(16.73,1.326)	(18.68,1.32)	
		1	(16.34,2.447)	(7.67,2.366)	(17.52,2.047)	17.7,2.044)	(17.66,2.037)	(17.62,2.024)	(17.14,1.818)	(15.06,1.481)	(16.73,1.465)	(18.6,1.398)	
		2	(16.32,2.385)	(7.72,2.265)	(17.7,1.992)	(17.66,1.986)	(17.6,1.968)	(17.54,1.967)	(17.5,1.962)	(17.18,1.851)	(17.96,1.807)	(15.4,1.521)	
		3	(7.56,2.72)	(16.06,2.047)	(15.86,1.906)	(15.34,1.813)	(17.28,1.779)	(17.12,1.722)	(16.84,1.49)	(14.44,1.454)	(17.7,1.426)	(18.46,1.269)	
8		None	(7.5,2.549)	(16.1,2.123)	(17.24,1.819)	(17.2,1.817)	(17.28,1.814)	(15.32,1.665)	(14.46,1.368)	(18.46,1.326)	(16.57,1.127)	(18.09,1.10)	
		1	(7.46,2.401)	(16.14,2.175)	(17.28,1.875)	(17.24,1.873)	(17.04,1.802)	(15.28,1.571)	(18.46,1.394)	(14.48,1.29)	(16.55,1.268)	(18.11,1.188)	
		2	(7.42,2.273)	(16.18,2.252)	(15.92,2.101)	(17.34,1.927)	(17.1,867)	(15.25,1.509)	(18.46,1.465)	(16.57,1.413)	(18.11,1.273)	(14.5,1.21)	
		3	(16.16,2.218)	(15.94,2.183)	(7.62,2.067)	(17.38,1.877)	(17.02,1.855)	(17.74,1.845)	(17.2,1.837)	(17.16,1.834)	(7.34,1.69)	(15.3,1.578)	
8		None	(7.19,3.119)	(7.5,2.645)	(15.64,2.055)	(15.9,1.83)	(17.42,1.644)	(17.02,1.641)	(16.98,1.636)	(17.06,1.635)	(14.18,1.632)		
		1	(7.18,3.158)	(7.48,2.292)	(7.42,2.272)	(15.66,2.005)	(15.96,1.853)	(17.08,1.732)	(17.04,1.727)	(15.16,1.653)	(17.44,1.629)	(16.62,1.617)	
		2	(7.17,3.156)	(15.68,1.963)	(16.04,1.906)	(17.1,1.813)	(16.64,1.689)	(17.44,1.644)	(15.14,1.562)	(18.16,1.384)	(14.16,1.29)	(16.35,1.285)	
		3	(7.16,3.134)	(16.08,1.999)	(15.7,1.963)	(17.14,1.87)	(16.64,1.792)	(17.4,1.702)	(15.12,1.502)	(18.14,1.467)	(16.35,1.413)	(17.83,1.322)	
	4	(7.15,2.643)	(15.72,2.036)	(16.04,1.968)	(17.2,1.837)	(7.56,1.808)	(17.56,1.743)	(16.68,1.727)	(15.13,1.547)	(18.18,1.529)	(18.14,1.527)		