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Adsorption properties of small gas molecules on $SnSe_2$ monolayer supported with Transition metal: First-principles calculations

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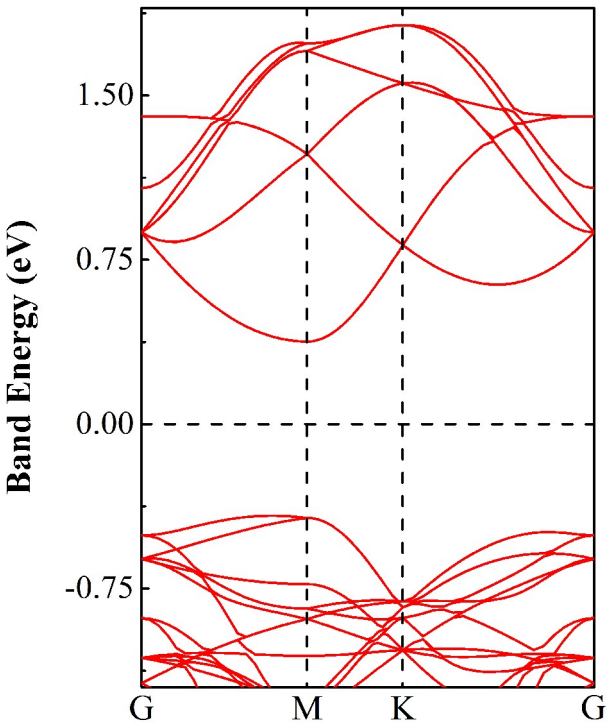

Fig. S1. The band structure of intrinsic $SnSe_2$.

Table S1. The relevant parameters of CH_4 gas molecule adsorbed on TMs supported $SnSe_2$ surface. The different adsorption configuration (Models), adsorption configuration of gas molecules (State), the adsorption energy of gas molecules (E_{ad} in eV), the distance between the gas molecules and the TM supported $SnSe_2$ (Height Å), the bond length (Å) and bond angle (°) of the gas molecules after adsorption, the charge transfer (Q in e).

Models	States	E_{ad} (eV)	Height (Å)	Bond length (Å)				Q(e)
				d_{C-Ha}	d_{C-Hb}	d_{C-Hc}	d_{C-Hd}	
	1P	-0.151	3.449	1.095	1.095	1.095	1.103	-0.004
Sc	2P	-0.356	2.789	1.107	1.095	1.105	1.095	-0.031
	3P	-0.400	2.643	1.104	1.104	1.104	1.097	-0.037
	1P	-0.146	3.464	1.095	1.095	1..095	1.105	-0.003
Ti	2P	-0.276	2.835	1.107	1.096	1.104	1.095	-0.014
	3P	-0.282	2.714	1.102	1.102	1.102	1.098	-0.021
	1P	-0.158	3.368	1.096	1.096	1.096	1.106	0.001
V	2P	-0.272	2.764	1.109	1.096	1.103	1.095	-0.005
	3P	-0.245	2.890	1.100	1.101	1.100	1.099	-0.008
	1P	-0.197	2.926	1.099	1.099	1.099	1.098	-0.002
Cr	2P	-0.231	2.769	1.108	1.096	1.103	1.096	-0.011
	3P	-0.146	3.362	1.096	1.096	1.096	1.106	-0.007
	1P	-0.137	3.397	1.096	1.096	1.096	1.105	0.001
Mn	2P	-0.195	3.012	1.103	1.096	1.101	1.096	0.001
	3P	-0.200	2.960	1.099	1.099	1.099	1.098	0.001
	1P	-0.132	3.420	1.096	1.096	1.096	1.103	-0.002
Fe	2P	-0.171	3.261	1.110	1.097	1.099	1.097	0.006
	3P	-0.171	3.142	1.098	1.099	1.099	1.098	0.002
	1P	-0.131	3.459	1.096	1.096	1.096	1.103	0.002
Co	2P	-0.158	3.363	1.099	1.097	1.098	1.097	0.006
	3P	-0.160	3.320	1.098	1.098	1.098	1.098	0.012
	1P	-0.132	3.494	1.096	1.096	1.096	1.101	0.003
Ni	2P	-0.162	3.372	1.099	1.097	1.098	1.097	0.007
	3P	-0.165	3.330	1.097	1.098	1.097	1.097	0.010
	1P	-0.125	3.551	1.097	1.097	1.097	1.100	0.004
Cu	2P	-0.155	3.398	1.099	1.097	1.099	1.097	0.009
	3P	-0.161	3.294	1.098	1.098	1.098	1.098	0.005

Table S2. The relevant parameters of H_2S gas molecule adsorbed on TMs supported $SnSe_2$ surface. The different adsorption configuration (Models), adsorption configuration of gas molecules (State), the adsorption energy of gas molecules (E_{ad} in eV), the distance between the gas molecules and the TM supported $SnSe_2$ (Height Å), the bond length (Å) and bond angle (°) of the gas molecules after adsorption, the charge transfer (Q in e).

Models	States	E_{ad} (eV)	Height (Å)	Bond length (Å)		Bond angle (°)	Q(e)
				d_{S-Ha}	d_{S-Hb}		
	1R	-0.797	2.789	1.354	1.354	92.397	-0.956
Sc	2R	-0.794	2.759	1.353	1.354	92.308	-0.087
	3R	-0.808	2.775	1.353	1.355	92.260	-0.080
	1R	-0.755	2.716	1.353	1.353	92.344	-0.088
Ti	2R	-0.783	2.660	1.353	1.354	92.407	-0.091
	3R	-0.784	2.675	1.354	1.354	92.276	-0.102
	1R	-0.813	2.585	1.355	1.354	92.334	-0.078
V	2R	-0.837	2.553	1.354	1.354	92.386	-0.108
	3R	-0.837	2.553	1.354	1.355	92.307	-0.111
	1R	-0.807	2.530	1.355	1.356	92.231	-0.147
Cr	2R	-0.819	2.515	1.354	1.355	92.323	-0.124
	3R	-0.819	2.510	1.354	1.355	91.984	-0.111
	1R	-0.714	2.545	1.354	1.354	92.265	-0.099
Mn	2R	-0.735	2.512	1.353	1.354	92.323	-0.124
	3R	-0.735	2.517	1.354	1.354	92.255	-0.139
	1R	-0.721	2.402	1.356	1.356	92.171	-0.109
Fe	2R	-0.749	2.383	1.355	1.356	92.203	-0.130
	3R	0.748	2.386	1.355	1.356	92.096	-0.153
	1R	-0.723	2.310	1.359	1.359	91.679	-0.082
Co	2R	-0.734	2.307	1.356	1.358	91.560	-0.181
	3R	-0.733	2.309	1.356	1.359	91.692	-0.166
	1R	-0.678	2.302	1.358	1.358	91.780	-0.098
Ni	2R	-0.690	2.300	1.356	1.357	91.758	-0.189
	3R	-0.687	2.301	1.355	1.357	91.612	-0.175
	1R	-0.520	2.422	1.354	1.353	92.245	-0.107
Cu	2R	-0.536	2.407	1.353	1.354	92.022	-0.174
	3R	-0.533	2.409	1.353	1.354	92.012	-0.165

Table S3. The relevant parameters of SO_2 gas molecule adsorbed on TMs supported $SnSe_2$ surface. The different adsorption configuration (Models), adsorption configuration of gas molecules (State), the adsorption energy of gas molecules (E_{ad} in eV), the distance between the gas molecules and the TM supported $SnSe_2$ (Height Å), the bond length (Å) and bond angle (°) of the gas molecules after adsorption, the charge transfer (Q in e).

Models	States	E_{ad} (eV)	Height (Å)	Bond length (Å)		Bond angle (°)	Q(e)
				d_{S-O1}	d_{S-O2}		
	1S	-1.613	2.757	1.546	1.546	102.660	0.623
Sc	2S	-0.322	2.703	1.456	1.458	121.284	0.279
	3S	-1.609	2.757	1.549	1.543	102.767	0.621
	1S	-1.199	2.737	1.466	1.595	111.726	0.474
Ti	2S	-0.427	2.528	1.455	1.457	120.387	0.287
	3S	-1.285	2.744	1.552	1.543	100.495	0.596
	1S	-0.563	2.395	1.454	1.453	119.644	0.224
V	2S	-0.561	2.393	1.453	1.454	119.632	0.269
	3S	-0.991	2.752	1.546	1.521	102.182	0.525
	1S	-0.497	2.369	1.452	1.452	119.982	0.235
Cr	2S	-0.496	2.372	1.451	1.452	119.844	0.190
	3S	-0.635	2.727	1.542	1.544	100.190	0.580
	1S	-0.403	2.292	1.454	1.454	119.607	0.243
Mn	2S	-0.409	2.287	1.453	1.455	119.685	0.290
	3S	-0.421	3.307	1.461	1.514	115.619	0.302
	1S	-0.680	2.153	1.453	1.453	118.190	0.233
Fe	2S	-0.678	2.152	1.453	1.454	118.149	0.176
	3S	-0.695	3.331	1.460	1.180	116.180	0.273
	1S	-0.149	3.719	1.449	1.449	118.887	0.038
Co	2S	-0.613	2.130	1.451	1.452	118.234	0.203
	3S	-0.523	3.264	1.499	1.457	117.162	0.227
	1S	-0.151	3.712	1.449	1.449	118.856	0.037
Ni	2S	-0.476	2.154	1.450	1.450	118.673	0.175
	3S	-0.390	3.268	1.487	1.453	117.600	0.150
	1S	-0.180	3.228	1.450	1.450	119.085	0.072
Cu	2S	-0.215	2.929	1.451	1.451	119.074	0.113
	3S	-0.282	3.381	1.478	1.453	117.559	0.147

Table S4. The relevant parameters of CO gas molecule adsorbed on TMs supported $SnSe_2$ surface. The different adsorption configuration (Models), adsorption configuration of gas molecules (State), the adsorption energy of gas molecules (E_{ad} in eV), the distance between the gas molecules and the TM supported $SnSe_2$ (Height Å), the bond length (Å) and bond angle (°) of the gas molecules after adsorption, the charge transfer (Q in e).

Models	**States**	E_{ad} **(eV)**	**Height (Å)**	**Bond length (Å)** d_{C-O}	**Q(e)**
	1T	-0.311	2.429	1.150	-0.002
Sc	2T	-0.625	2.424	1.143	0.041
	3T	-0.313	2.446	1.150	0.007
	1T	-0.818	2.203	1.151	0.136
Ti	2T	-0.817	2.205	1.150	0.128
	3T	-0.225	2.434	1.150	0.009
	1T	-1.152	2.030	1.151	0.195
V	2T	-1.154	2.026	1.156	0.125
	3T	-0.258	2.261	1.153	0.065
	1T	-1.093	2.003	1.153	0.103
Cr	2T	-1.095	2.006	1.153	0.147
	3T	-0.207	2.335	1.150	0.024
	1T	-0.925	1.929	1.156	0.169
Mn	2T	-0.926	1.192	1.156	0.210
	3T	-0.120	2.935	1.145	0.011
	1T	-0.093	3.492	1.144	0.018
Fe	2T	-1.507	1.788	1.163	0.090
	3T	-0.101	2.996	1.145	0.011
	1T	-0.096	3.538	1.144	0.015
Co	2T	-1.423	1.774	1.160	0.021
	3T	-0.091	2996	1.144	0.012
	1T	-0.098	3.559	1.144	0.015
Ni	2T	-1.229	1.788	1.156	0.042
	3T	-0.091	2.996	1.144	0.011
	1T	-0.097	3.652	1.144	0.013
Cu	2T	-0.632	1.889	1.148	-0.032
	3T	-0.090	3.150	1.144	0.011

Table S5. The relevant parameters of H_2O gas molecule adsorbed on TMs supported $SnSe_2$ surface. The different adsorption configuration (Models), adsorption configuration of gas molecules (State), the adsorption energy of gas molecules (E_{ad} in eV), the distance between the gas molecules and the TM supported $SnSe_2$ (Height Å), the bond length (Å) and bond angle (°) of the gas molecules after adsorption, the charge transfer (Q in e).

Models	States	E_{ad} (eV)	Height (Å)	Bond length (Å)		Bond angle (°)	Q(e)
				d_{Ha-O}	d_{Hb-O}		
	1U	-1.093	2.251	0.977	0.977	106.940	-0.060
Sc	2U	-1.068	2.231	0.976	0.974	108.643	-0.062
	3U	-1.071	2.235	00.977	0.974	108.526	-0.059
	1U	-0.964	2.215	0.978	0.978	107.244	-0.056
Ti	2U	-0.918	2.195	0.975	0.974	108.928	-0.068
	3U	-0.968	2.214	0.979	0.978	107.090	-0.056
	1U	0.899	2.169	0.977	0.978	107.476	-0.058
V	2U	-0.752	2.170	0.978	0.978	107.286	-0.057
	3U	-0.860	2.163	0.974	0.974	108.961	-0.062
	1U	-0.816	2.171	0.977	0.978	106.936	-0.041
Cr	2U	-0.816	2.171	0.978	0.978	106.682	-0.061
	3U	-0.816	2.167	0.978	0.978	106.786	-0.058
	1U	-0.745	2.173	0.977	0.978	106.926	-0.054
Mn	2U	-0.699	2.145	0.974	0.974	109.344	-0.074
	3U	-0.748	2.179	0.978	0.978	106.615	-0.052
	1U	-0.667	2.160	0.978	0.978	106.731	-0.070
Fe	2U	-0.668	2.156	0.978	0.978	106.637	-0.055
	3U	-0.668	2.156	0.978	0.978	106.614	-0.049
	1U	-0.563	2.162	0.978	0.978	106.207	-0.064
Co	2U	-0.562	2.160	0.979	0.979	106.071	-0.047
	3U	-0.561	2.162	0.978	0.978	106.120	-0.047
	1U	-0.510	2.153	0.978	0.978	106.028	-0.048
Ni	2U	-0.509	2.152	0.978	0.978	105.990	-0.067
	3U	-0.509	2.154	0.978	0.978	106.029	-0.043
	1U	-0.454	2.199	0.977	0.978	105.894	-0.068
Cu	2U	-0.455	2.198	0.978	0.978	105.736	-0.059
	3U	-0.454	2.192	0.978	0.978	105.901	-0.043

Table S6. The relevant parameters of NO gas molecule adsorbed on TMs supported $SnSe_2$ surface. The different adsorption configuration (Models), adsorption configuration of gas molecules (State), the adsorption energy of gas molecules (E_{ad} in eV), the distance between the gas molecules and the TM supported $SnSe_2$ (Height Å), the bond length (Å) and bond angle (°) of the gas molecules after adsorption, the charge transfer (Q in e).

Models	States	E_{ad} (eV)	Height (Å)	Bond length (Å) d_{N-O}	Q(e)
	1Y	-1.137	2.166	1.245	0.465
Sc	2Y	-1.459	2.044	1.199	0.423
	3Y	-1.016	2.014	1.232	0.419
	1Y	-1.604	1.897	1.266	0.524
Ti	2Y	-1.834	1.904	1.193	0.346
	3Y	-1.127	1.942	1.221	0.341
	1Y	-2.432	1.752	1.193	0.320
V	2Y	-2.433	1.752	1.193	0.371
	3Y	-0.941	1.894	1.204	0.263
	1Y	-2.315	1.669	1.189	0.380
Cr	2Y	-2.316	1.699	1.189	0.247
	3Y	-0.492	1.990	1.198	0.185
	1Y	-2.276	1.681	1.185	0.328
Mn	2Y	-2.276	1.682	1.185	0.196
	3Y	-0.095	2.968	1.174	0.032
	1Y	-2.423	1.663	1.177	0.188
Fe	2Y	-2.423	1.662	1.177	0.246
	3Y	-0.930	1.804	1.187	0.259
	1Y	-2.161	1.649	1.173	0.102
Co	2Y	-2.160	1.649	1.173	0.179
	3Y	0.089	3.002	1.167	-0.031
	1Y	-1.187	1.688	1.169	0.025
Ni	2Y	-1.205	1.170	1.171	0.112
	3Y	-0.163	2.748	1.169	-0.016
	1Y	-0.630	1.976	1.177	0.096
Cu	2Y	-0.124	3.005	1.167	-0.025
	3Y	-0.092	3.196	1.166	-0.041