

First-Principles Insights into Highly Sensitive and Reusable MoS₂ Monolayers for Heavy Metal Detection

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Table S1: Temperature-dependent recovery time of MoS₂ for heavy metal adsorption

Heavy metal	Temperature	Recovery time
As	298K	9.67 s
As	398K	2.96×10^{-3} s
As	498K	2.34×10^{-5} s
Cd	298K	3.54×10^{-6} s
Cd	398K	4.49×10^{-8} s
Cd	498K	3.29×10^{-9} s
Hg	298K	1.56×10^{-7} s
Hg	398K	4.33×10^{-9} s
Hg	498K	5.07×10^{-10} s
Pb	298K	2.21×10^{10} s
Pb	398K	3.02×10^4 s
Pb	498K	9.32 s

Table S2: Comparison between this work with previous reports

Sensing material	Heavy metal	Adsorption energy E_{ad} (eV)	Recovery time, temperature	Sensitivity, bias voltage ^a	Ref
<i>MoS₂</i>	As	-0.827	9.67 s, 298K	126452.28%,0.2V	This work
<i>SnS</i>	As	-1.599	2.99 s, 598K	43286%,0.3V	[1]
<i>SnSe</i>	As	-0.663	0.016 s, 298K	384467%,0.2V	[2]
<i>graphene</i>	As	-1.39		36.06%, 0.6V	[3]
<i>graphene -H₂O</i>	As	-0.97			[3]
<i>boron functionalized graphene</i>	As	-2.63			[4]
<i>boron functionalized graphene-H₂O</i>	As	-1.91			[4]
<i>graphene-H₂O</i>	As	-1.73		19%, 0.2V	[5]
<i>Cu-B-graphene-H₂O</i>	As	-3.43		25%, 0.2V	[5]
<i>Cu-N-graphene-H₂O</i>	As	-3.93		55%, 0.2V	[5]
<i>zigzag ZnO nanoribbons</i>	As			3.52×10^7 , 0.3V	[6]
<i>MoS₂</i>	Cd	-0.446	3.54×10^{-6} s, 298K	1862.67%,0.8V	This work
<i>SnS</i>	Cd	-0.384	31.2 μ s, 298K	442%,0.5V	[1]
<i>SnSe</i>	Cd	-0.427	1.67×10^{-6} s, 298K	1462%,0.1V	[2]
<i>graphene</i>	Cd	-0.23			[3]
<i>graphene -H₂O</i>	Cd	-0.31			[3]
<i>Epitaxial graphene</i>	Cd	0.217			[7]
<i>Epitaxial graphene-H₂O</i>	Cd	0.293			[7]
<i>zinc-oxide nanotube</i>	Cd	-1.30			[8]
<i>zinc-oxide graphene-like structure</i>	Cd	-0.24			[8]
<i>single vacancy graphene</i>	Cd	-0.409			[9]
<i>graphene/SiC</i>	Cd			8.5702×10^{-8} , 1V	[10]
<i>MoS₂</i>	Hg	-0.366	1.56×10^{-7} s, 298K	427.71%,0.5V	This work
<i>SnS</i>	Hg	-0.473	9.986 μ s, 298K	10%,0.5V	[1]
<i>SnSe</i>	Hg	-0.278	5.03×10^{-9} s, 298K	1791%, 0.1V	[2]
<i>graphene</i>	Hg	-0.26			[3]
<i>graphene -H₂O</i>	Hg	-0.32			[3]
<i>Epitaxial graphene</i>	Hg	0.246			[7]
<i>Epitaxial graphene-H₂O</i>	Hg	0.384			[7]
<i>graphene/SiC</i>	Hg			3.868×10^{-8} , 1V	[10]
<i>Ti₂C</i>	Hg	-0.735	28.8 s,400K		[11]
<i>1T-MoS₂</i>	Hg	-1.091			[12]
<i>Pd₂-pyridine-like N-graphene</i>	Hg	-1.02			[13]
<i>MoS₂</i>	Pb	-1.380	9.32 s, 498K	83438.90%,0.4V	This work
<i>SnS</i>	Pb	-1.766	76.44 s, 598K	368860%, 0.5V	[1]
<i>SnSe</i>	Pb	-1.441	38.3 s, 498K	26160%,0.2V	[2]

graphene	Pb	-0.91		34.42%, 0.6V	[3]
graphene -H ₂ O	Pb	-0.97			[3]
zigzag ZnO nanoribbons	Pb			2.86×10 ⁷ , 0.2V	[6]
Epitaxial graphene	Pb	0.641			[7]
Epitaxial graphene-H ₂ O	Pb	1.57			[7]
graphene/SiC	Pb			13600%, 1V	[10]
B dope- graphene	Pb	-2.40	1.4×10 ¹⁴ μs,600K		[14]
N dope- graphene	Pb	-1.01	302 μs,600K		[14]
B dope -graphene-H ₂ O	Pb	-1.73	3.31×10 ⁸ μs,600K	16.12%,0.15V	[14]
N dope -graphene-H ₂ O	Pb	-0.95	8.63 μs,600K	329.04%,0.15V	[14]

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