Density Functional Theory Provides Insights into β-SnSe Monolayers as a Highly Sensitive and Recoverable Ozone Sensing Material

Jiayin Wu [1,2], Zongbao Li [3,4,*], Tongle Liang [5], Qiuyan Mo [6], Jingting Wei [1], Bin Li [1] and Xiaobo Xing [2,*]

[1] Department of Engineering Technology, Guangdong Open University, Guangzhou 510091, China; wujiayin@m.scnu.edu.cn (J.W.); jtwei@gdrtvu.edu.cn (J.W.); bli@gdrtvu.edu.cn (B.L.)
[2] Centre for Optical and Electromagnetic Research, South China Academy of Advanced Optoelectronics, South China Normal University, Guangzhou 510006, China
[3] Ministry of Education Key Laboratory of Textile Fiber Products, School of Materials Science and Engineering, Wuhan Textile University, Wuhan 430220, China
[4] School of Materials and Chemistry Engineering, Tongren University, Tongren 554300, China
[5] School of Artificial Intelligence, Guangdong Vocational College of Post and Telecom, Guangzhou 510630, China; liangtongle@gupt.edu.cn
[6] Big Data Engineering College, Kaili University, Kaili 556011, China; 2014020983@kluniv.edu.cn
* Correspondence: zongbaoli1982@163.com (Z.L.); xingxiaobo@scnu.edu.cn (X.X.)

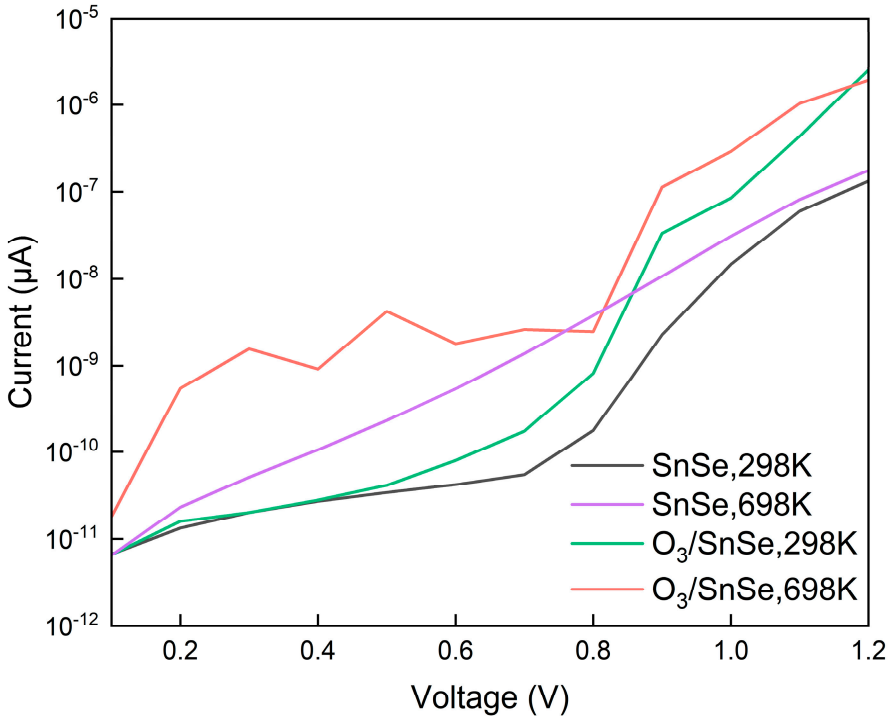


Figure S1. The sensitivity for intrinsic and O3-adsorbed SnSe monolayers at temperatures from 298 to 698 K

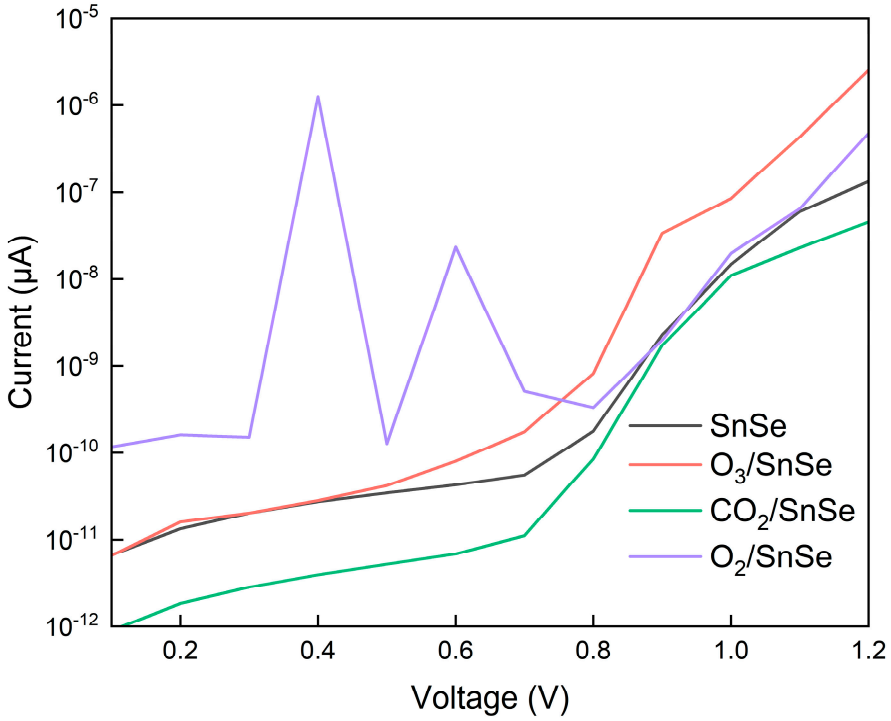


Figure S2. Current-voltage characteristics of SnSe monolayers without adsorbed gas molecules and with adsorbed O_2, O_3, and CO_2

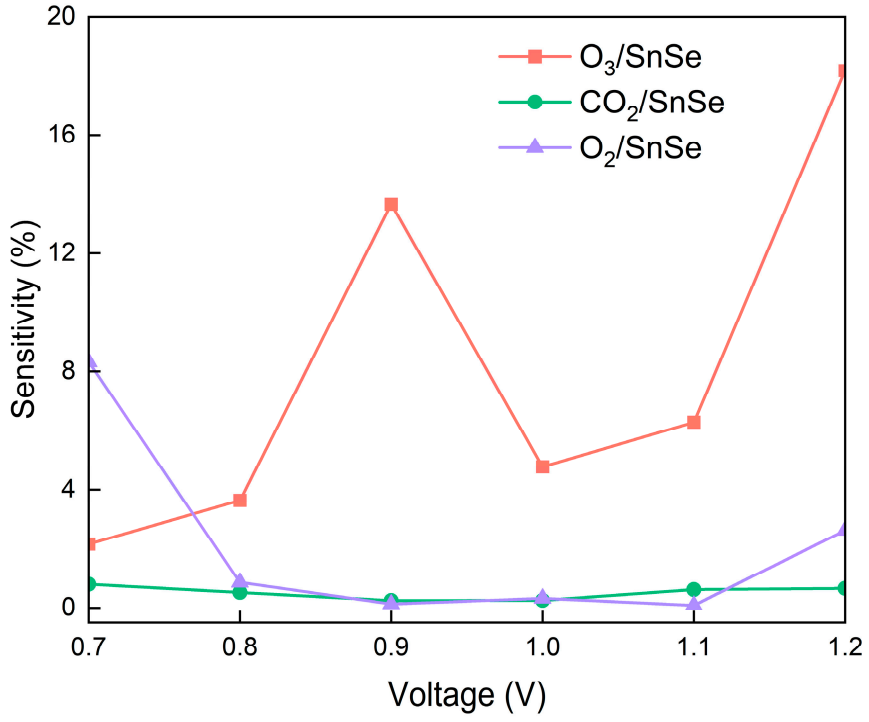


Figure S3. Voltage-dependent sensitivity curves of SnSe monolayers with adsorbed O_2, O_3, and CO_2 molecules

TABLE SI

Comparison between this work with previous reports

Sensing material	Adsorption energy E_{ad}(eV)	Charge transfer(e)	Recovery time, temperature	Sensitivity	Ref
SnSe	-1.826	0.881	1.53s, 698K	1817.57%	This work
MoS_2	-0.36	0.126	1.23×10^{-7} s, 298K[1]		[1]
SnS	-1.25	0.78	0.45s, 498K[1]		[2]
stanene	-2.06	0.557	74.79s, 698K[1]		[3]
B-doped stanene	-3.15	0.548	5.55×10^{9} s, 698K[1]		[3]
BN fullerene-like nano-cage	-1.8	-0.5	0.99s, 698K[1]		[4]
B--decorated $B_{12}N_{12}$ nanocages	-4.10 [2]	0.789			[5]
AlN nanotube	-1.88		3.75s, 698K[1]		[6]
graphene oxide				860%	[7]

[1] The recovery time was determined by extracting the adsorption energy data from the corresponding references and substituting it into Equation 4.

[2] The adsorption energy data from the references have been converted from kJ/mol to eV for consistency.

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