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Effect of Cu intercalation on humidity sensing properties of Bi_2Se_3 topological insulator single crystals

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Supplementary Information

Table 1: Structural parameters obtained from a Rietveld refinement of room temperature powder x-ray patterns shown in Fig. 3.

Sample	Atom	X	Y	Z	Occupancy
Bi_2Se_3	**Bi**	**0**	**0**	**0.40276**	**0.09211**
***a*=*b*=4.141±0.003Å**	**Se1**	**0**	**0**	**0**	**0.08892**
***c*=28.665±0.002Å**	**Se2**	**0**	**0**	**0.20841**	**0.18040**
$Cu_{0.13}Bi_2Se_3$	**Bi**	**0**	**0**	**0.40142**	**0.08779**
***a*=*b*=4.141±0.002Å**	**Se1**	**0**	**0**	**0**	**0.03658**
***c*=28.713±0.003Å**	**Se2**	**0**	**0**	**0.20091**	**0.08305**
$Cu_{0.25}Bi_2Se_3$	**Bi**	**0**	**0**	**0.40089**	**0.08478**
***a*=*b*=4.141±0.004Å**	**Se1**	**0**	**0**	**0**	**0.01031**
***c*=28.734±0.003Å**	**Se2**	**0**	**0**	**0.20024**	**0.02358**

Table 2: Hysteresis values of pure and Cu intercalated Bi_2Se_3 ($Cu_0Bi_2Se_3$, $Cu_{0.13}Bi_2Se_3$ and $Cu_{0.25}Bi_2Se_3$) at different levels of %RH.

RH%	**Bi_2Se_3**	**$Cu_{0.13}Bi_2Se_3$**	**$Cu_{0.25}Bi_2Se_3$**
8	0.00177	0.00021	0.00050
33	0.00188	0.00966	0.00117
43	0.00212	0.00318	0.00133
52	0.00070	0.00546	0.00104
63	0.00377	0.00028	0.00084
75	0.00396	0.00693	0.00079
86	0.00115	0.00481	0.00048
97	0.00041	0.00021	0.00023

Table 3: Freundlich adsorption isotherm model results, including adsorption capacity (*k*), adsorption strength (α), and R^2 values vs. the experimental data for humidity sensing using Bi_2Se_3, $Cu_{0.13}Bi_2Se_3$ and $Cu_{0.25}Bi_2Se_3$.

Sample	**Low RH Regime**			**High RH Regime**		
	k	***α***	***R^2***	***k***	***α***	***R^2***
Bi_2Se_3	**1.03±0.06**	**1.72±0.14**	**0.96**	**1.32±0.27**	**0.40±0.04**	**0.97**
$Cu_{0.13}Bi_2Se_3$	**2.31±0.29**	**1.22±0.16**	**0.87**	**1.46±0.31**	**0.66±0.09**	**0.92**
$Cu_{0.25}Bi_2Se_3$	**4.3±0.19**	**0.91±0.08**	**0.92**	**3.03±0.16**	**0.87±0.02**	**0.95**

Table 4: Comparative analysis of Cu intercalated Bi_2Se_3 TI humidity sensor in terms of linear range, sensitivity, response and recovery time with available literatures.

Material	Linear Range (%)	Sensitivity	Response/ Recovery Time (s)	Reference
ZnO nanowires	25 to 90	184	NA	1
MoS_2 film	13.3 to 83.5	16.08(p-type) 89.66(n-type)	55s/288s(p-type) 174s/345s(n-type)	2
SnO_2:Sn composite thin film	11 to 95	265	80s/140s	3
CuO nanowires	20 to 90	12.72%	NA	4
Porous titania ceramics	11 to 95	$\sim 10^4$	32s/131s	5
ZnO nanosheets	12 to 96	220	600s/3s	6
Sn-doped ZnO nanorod Arrays	40 to 90	3.41	230s/30s	7
ZnO nanorods	33 to 95	61.23	NA	8
SnO_2 Nanowire	5 to 85	32	120s/20s	9
WS_2/WSe_2 Nanohybrids	40 to 80	57	40s/65s	10
Fe_2O_3/SiO_2 composites	11 to 95	10^4	20s/40s	11
WS_2 nanosheets	40 to 80	37.5	13s/17s	12
NiO–SnO_2 nanofibers	0 to 100	83	22s/44s	13
Polyaniline/WS_2 composite	10 to 97	88.46	56s/70s	14
rGO/MoS_2 hybrid composites	10 to 90	49	17s/474s	15
Single crystalline ZnO nanowire	10 to 90	88	60s/3s	16
Co doped mesoporous TiO_2	9 to 90	10^5	24s/400s	17

WS_2/GO Nanohybrids	40 to 80	0.044/%RH	25s/29s	18
TiO_2 nanotubes	11 to 95	~57	100s/190s	19
TiO_2 nanowires /Nafion	12 to 97	>1000	<120s/<120s	20
TiO_2 thin film	11 to 97	~10^2	10s/176s	21
ZnO nanocrystals	5 to 85	150	50s/6s	22
graphene/TiO_2 composites	12 to 90	10^2	128s/68s	23
WO_3-SnO_2 nanospheres	35 to 98	16.2	8s/29s	24
MoS_2 Thin Film	25 to 40	5.5	250s/250s	25
MoS_2 Nanosheets	10 to 60	~3	9s/17s	26
WS_2 spherical nanoparticle	11 to 97	469	12s/13s	27
VS_2 nanosheets	0 to 100	~325	40s/50s	28
SnSe nanorods	11-97	~100	68/149s	29
$Zn_{1-x}Ni_xO$ nanostructures	33-97	152	27/3 s	30
$CoFe_2O_4$ nanoparticles	8-97	~590	25/2.6 s	31
$Cu_xBi_2Se_3$	*8-97*	*849*	*24 s/25 s*	*This work*

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