Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Oxygen Induced Degradation in Electronic Properties of Thin-layer InSe

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Table S1 Full title of acronyms in manuscript

Acronyms	Full title
HSE	Heyd-Scuseria-Emzerhof
DFT	Density Functional Theory
PL	Photoluminescence
TSS	Transition States Search
PBE	Perdew-Burke-Ernzerhof
GGA	Generalized Gradient Approximation
DOS	Density of States
CBE	Conduction Band Edge
VBE	Valence Band Edge
CBM	Conduction Band Minimum
VBM	Valence Band Maximum
DP	Deformation Potential
e	Electron
h	Hole

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Table S2 In-plane stiffness C_{2D}, effective mass m^*, and deformation potential E_1 along the a_0 and b_0 directions in 2D monolayer InSe containing single O atom.

Position (O atom)		B_m	
Carrier type	C_{2D}(N/m)	m^*(m_e)	E_1(eV)
e (a)	75.93	0.21	-5.06
h (a)	75.93	2.52	4.7
e (b)	69.42	0.21	-6.6
h (b)	69.42	2.52	5.24
Position (O atom)		I_m1	
Carrier type	C_{2D}(N/m)	m^*(m_e)	E_1(eV)
e (a)	69.25	0.21	16.30
h (a)	69.25	1.43	23.81
e (b)	69.98	0.21	13.14
h (b)	69.98	1.43	15.06
Position (O atom)		I_m2	
Carrier type	C_{2D}(N/m)	m^*(m_e)	E_1(eV)
e (a)	69.27	0.21	-87.9
h (a)	69.27	2.64	-81.1
e (b)	70.67	0.21	-60.1
h (b)	70.67	2.64	-53.5
Position (O atom)		S_m	
Carrier type	C_{2D}(N/m)	m^*(m_e)	E_1(eV)
e (a)	66.67	0.22	3.08
h (a)	66.67	3.34	4.84
e (b)	66.68	0.22	3.48
h (b)	66.68	3.34	5.19

Table S3 In-plane stiffness C_{2D}, effective mass m^*, and deformation potential E_1 along the a_0 and b_0 directions in 2D bilayer InSe containing O atoms.

Position (O atom)		B_b	
Carrier type	C_{2D}(N/m)	$m^*(m_e)$	E_1(eV)
e (a)	135.88	0.18	-5.66
h (a)	135.88	0.87	1.42
e (b)	144.18	0.18	-5.04
h (b)	144.18	0.87	1.82
Position (O atom)		I_b1	
Carrier type	C_{2D}(N/m)	$m^*(m_e)$	E_1(eV)
e (a)	136.39	0.17	-5.8
h (a)	136.39	0.85	1.66
e (b)	140.57	0.17	-6.34
h (b)	140.57	0.85	2.52
Position (O atom)		I_b2	
Carrier type	C_{2D}(N/m)	$m^*(m_e)$	E_1(eV)
e (a)	137.87	0.17	-3.42
h (a)	137.87	0.86	3.58
e (b)	137.20	0.17	-3.36
h (b)	137.20	0.86	3.58
Position (O atom)		S_b1	
Carrier type	C_{2D}(N/m)	$m^*(m_e)$	E_1(eV)
e (a)	135.20	0.19	-4.76
h (a)	135.20	0.87	1.16
e (b)	135.20	0.19	-5.02
h (b)	135.20	0.87	0.74
Position (O atom)		S_b2	
Carrier type	C_{2D}(N/m)	$m^*(m_e)$	E_1(eV)
e (a)	135.33	0.20	-5.3
h (a)	135.33	0.98	2.4
e (b)	135.33	0.20	-5.26
h (b)	135.33	0.98	2.6
Position (O atom)		$2I_b2$	
Carrier type	C_{2D}(N/m)	$m^*(m_e)$	E_1(eV)
e (a)	140.20	0.18	-5.34
h (a)	140.20	0.90	1.44
e (b)	138.66	0.18	-4.28
h (b)	138.66	0.90	2.12

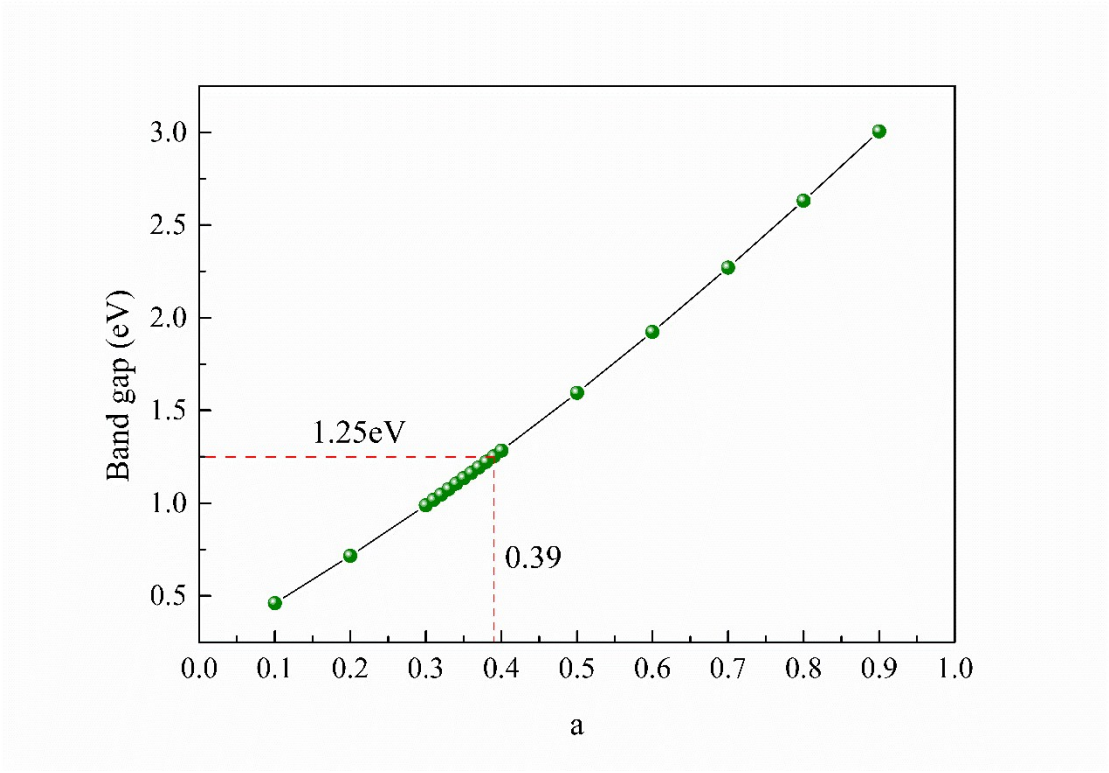

Fig. S1 The relationship between mixing parameter α and bandgap of bulk InSe

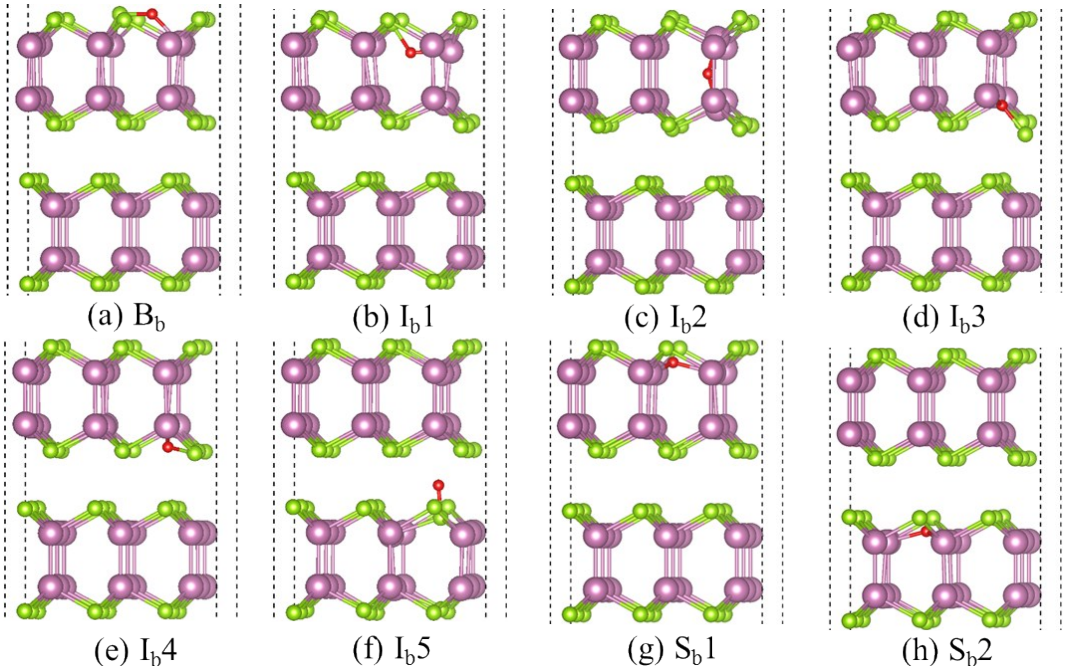

Fig. S2 Adsorbed structures of O atom on different sites: (a) B_b, (b) I_b1, (c) I_b2, (d) I_b3, (e) I_b4 and (f) I_b5, and substituted structures of (g) S_b1 and (h)S_b2.

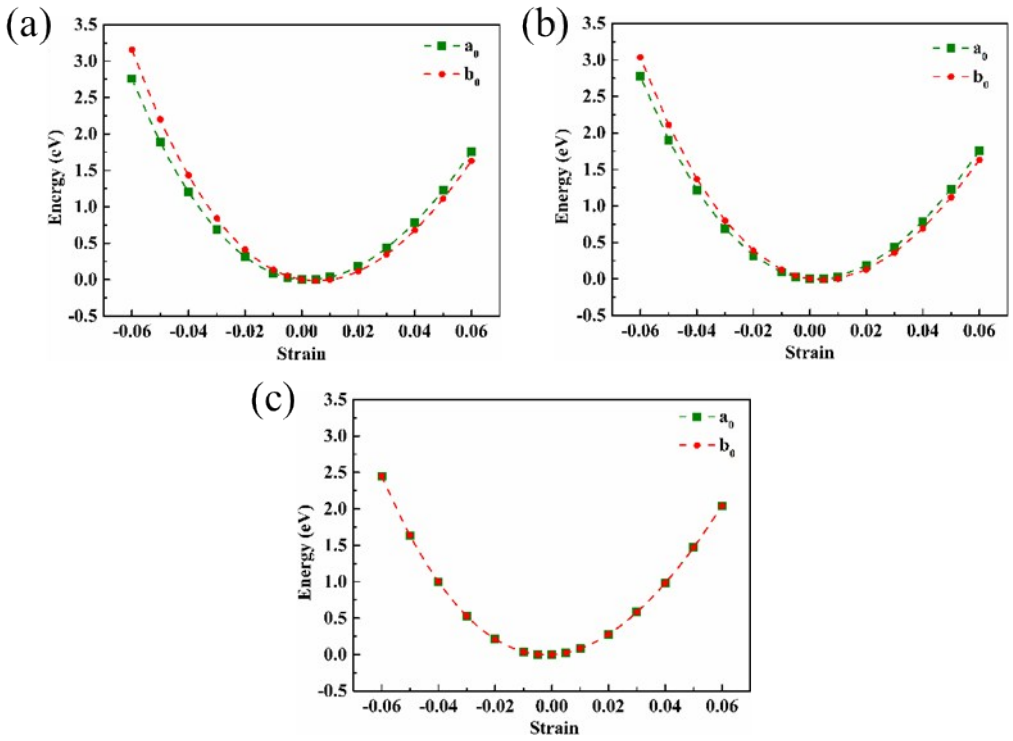

Fig. S3 Energy-strain relationships along the a_0 and b_0 directions of bilayer InSe (a) adsorbed structures of O atom on B_b site, (b) inserted O atom in $I_b1$site and (c) substituted structure of Se by O atom at S_b2 site.

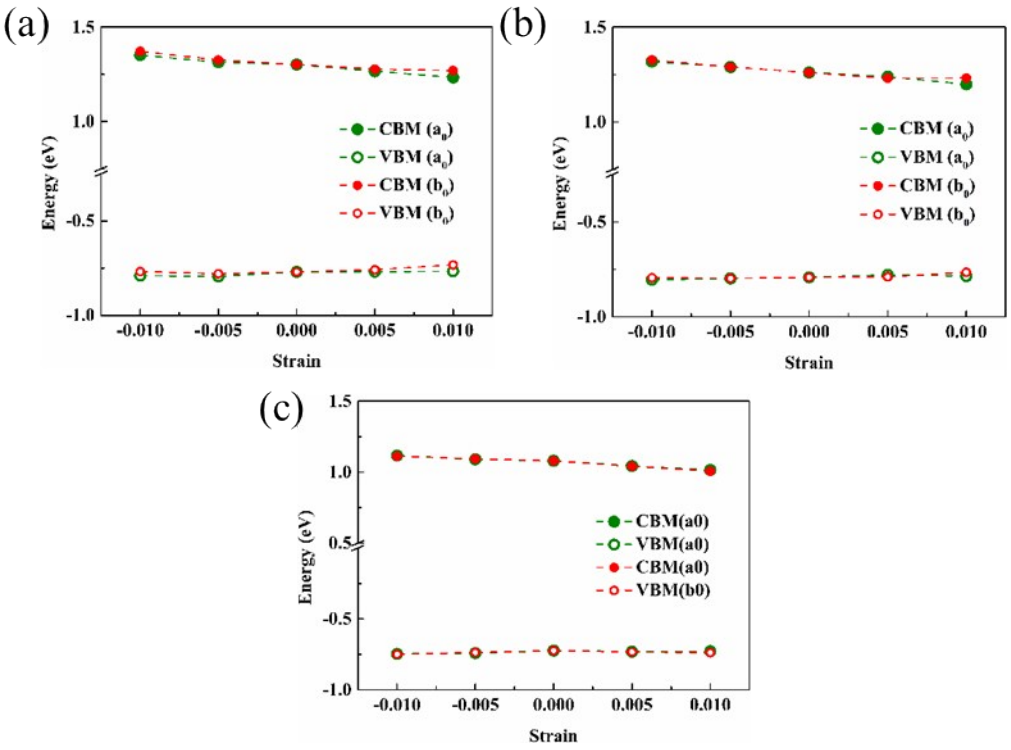

Fig. S4 Shifts of CBM and VBM under uniaxial strain along a_0 and b_0 directions of monolayer InSe (a) adsorbed structures of O atom on B_b site, (b) inserted O atom in $I_b1$site and (d) substituted structure of Se by O atom at S_b2 site.

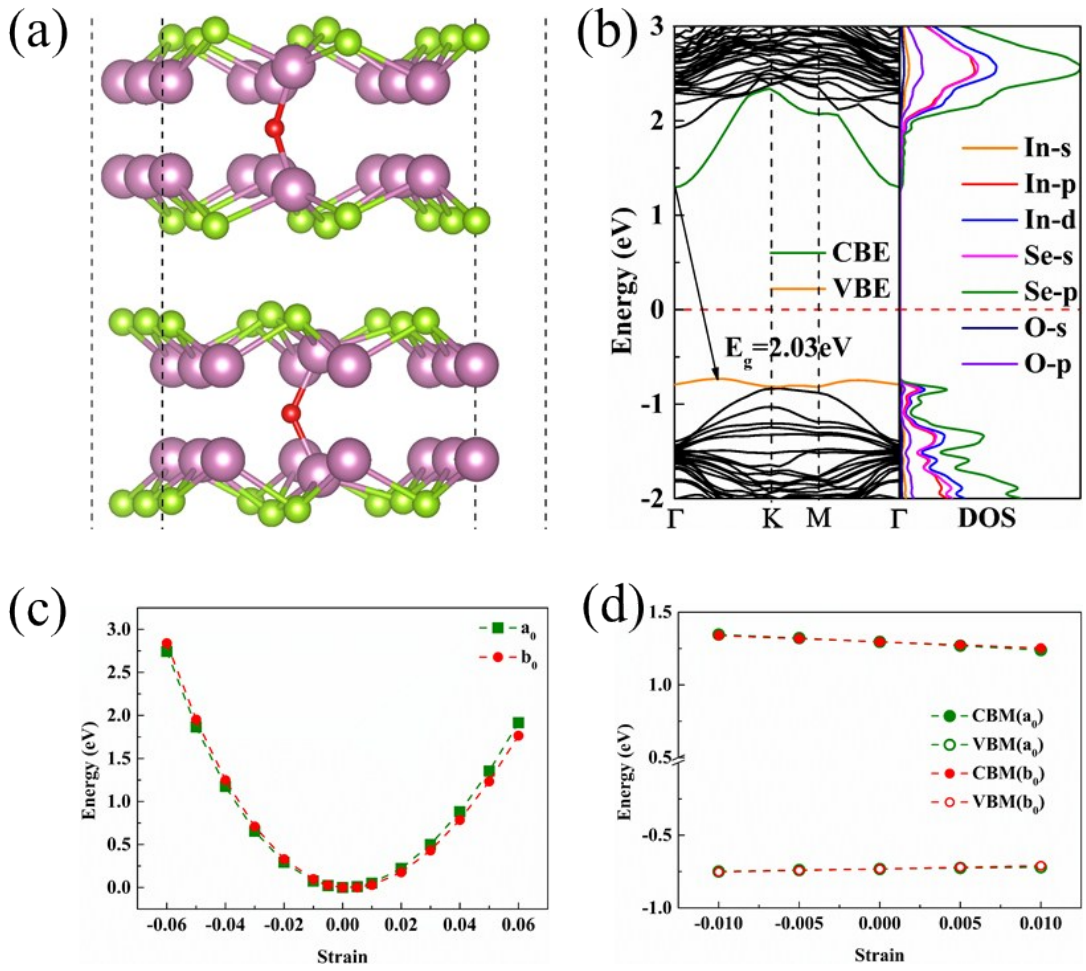

Fig.S5 (a) Optimized structure of bilayer InSe inserted O atom into I_b2 site of each layer and corresponding (b) Electronic band structure and density of states plots. The Fermi level is located at energy zero. (c) Energy-strain relationship and (d) shifts of CBM and VBM under uniaxial strain along a_0 and b_0 direction of bilayer InSe inserted O atom into I_b2 site of each layer.