Supporting Information of

Single Atom Modified Two Dimensional Bismuthene for Toxic Gases Detection

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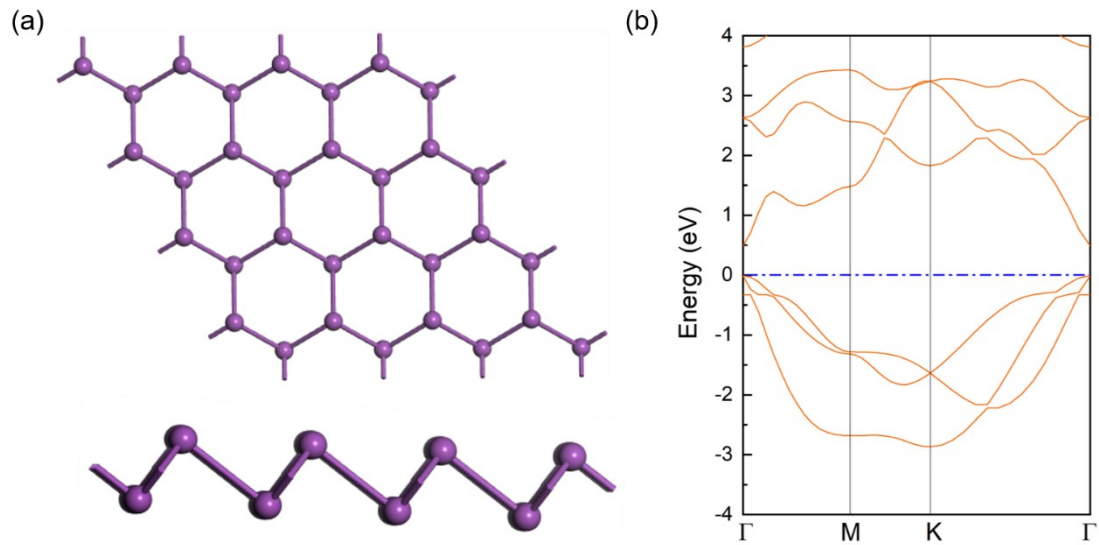*Correspondence to: Jinjin Li (lijinjin@sjtu.edu.cn)

Figure S1. (a) Top view and side view of the optimized pristine bBi. (b) Band structure of the pristine bBi, the blue dotted line presents the Fermi level.
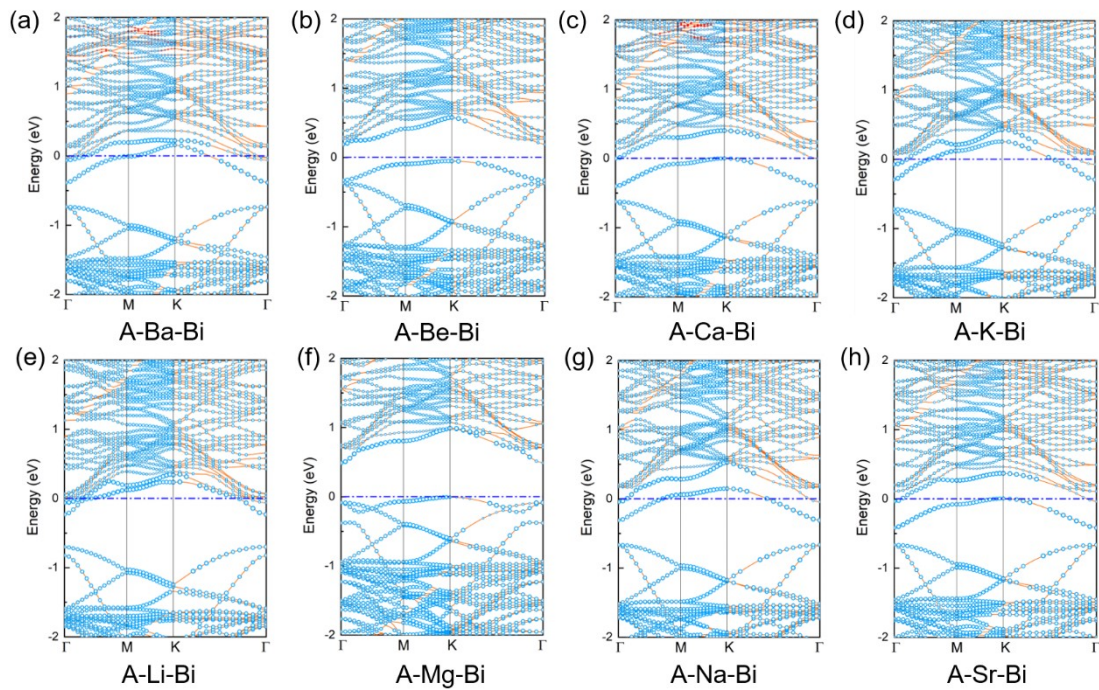

Figure S2. The band structures of A-M-Bi (M = Ba, Be, Ca, K, Li, Mg, Na, S), the blue dotted line presents the Fermi level.
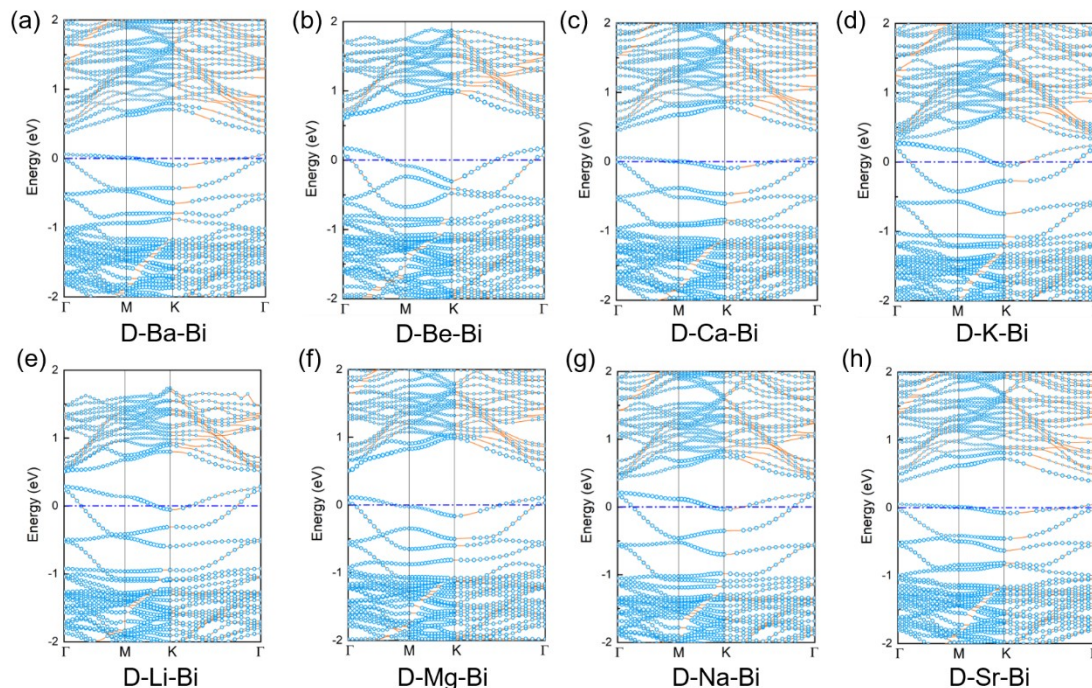
Figure S3. The band structures of D-M-Bi (M = Ba, Be, Ca, K, Li, Mg, Na, S), the blue dotted line presents the Fermi level.

Table S1 Results of the charge transfer from A-M-Bi to H_2S.

System	ΔQ (e)	System	ΔQ (e)
A-Ba-Bi	-0.0151	A-K-Bi	-0.0327
A-Be-Bi	0.1810	A-Mg-Bi	0.0580
A-Ca-Bi	0.0100	A-Na-Bi	-0.0175
A-Li-Bi	0.0169	A-Sr-Bi	-0.0037

Table S2 The work function of A-M-Bi ($W_{\text{A-M-Bi}}$), A-M-Bi with adsorbed H_2S ($W_{\text{A-H2S}}$) and the difference of work functions (ΔW).

System	$W_{\text{A-M-Bi}}$ (eV)	$W_{\text{A-M-Bi}}$ (eV)	ΔW (eV)
A-Ba-Bi	3.1521	3.0224	-0.1297
A-Be-Bi	3.6307	3.5213	-0.1094
A-Ca-Bi	3.3842	3.2496	-0.1346
A-Li-Bi	3.3124	3.2167	-0.0957
A-K-Bi	3.1303	2.9912	-0.1391
A-Mg-Bi	3.9427	3.8299	-0.1128
A-Na-Bi	3.2754	3.1335	-0.1419
A-Sr-Bi	3.2842	3.1034	-0.1808

Table S3 Results of the charge transfer from D-M-Bi to H_2S.

System	ΔQ (e)	System	ΔQ (e)
D-Ba-Bi	0.0052	D-K-Bi	-0.0061

D-Be-Bi	0.0008	D-Mg-Bi	0.0392
D-Ca-Bi	-0.0296	D-Na-Bi	-0.0297
D-Li-Bi	0.0067	D-Sr-Bi	0.0423

Table S4 The work function of D-M-Bi($W_{\text{D-M-Bi}}$), D-M-Bi with adsorbed H_2S ($W_{\text{D-M-Bi}}$) and the difference of work functions (ΔW).

System	$W_{\text{D-M-Bi}}$ (eV)	$W_{\text{D-M-Bi}}$ (eV)	ΔW (eV)
D-Ba-Bi	3.7355	3.4441	-0.2914
D-Be-Bi	4.0217	3.7667	-0.255
D-Ca-Bi	3.8488	3.4858	-0.363
D-Li-Bi	3.8454	3.5096	-0.3358
D-K-Bi	3.6267	3.3889	-0.2378
D-Mg-Bi	3.9273	3.636	-0.2913
D-Na-Bi	3.7234	3.4482	-0.2752
D-Sr-Bi	3.7898	3.516	-0.2738