

## Supplementary Information

### Two-Dimensional Borocarbonitrides for Photocatalysis and Photovoltaics

*Wei Zhang,<sup>\*,†,‡</sup> Changchun Chai,<sup>†</sup> Qingyang Fan,<sup>§</sup> Yintang Yang,<sup>†</sup> Minglei Sun,<sup>\*,||</sup> Maurizia*

*Palumbo,<sup>⊥</sup> and Udo Schwingenschlöggl<sup>\*,||</sup>*

<sup>†</sup>School of Microelectronics, Xidian University, Xi'an 710071, China

<sup>‡</sup>Beijing Institute of Astronautical Systems Engineering, Beijing 100076, China

<sup>§</sup>College of Information and Control Engineering, Xi'an University of Architecture and Technology, Xi'an 710055, China

<sup>||</sup>Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

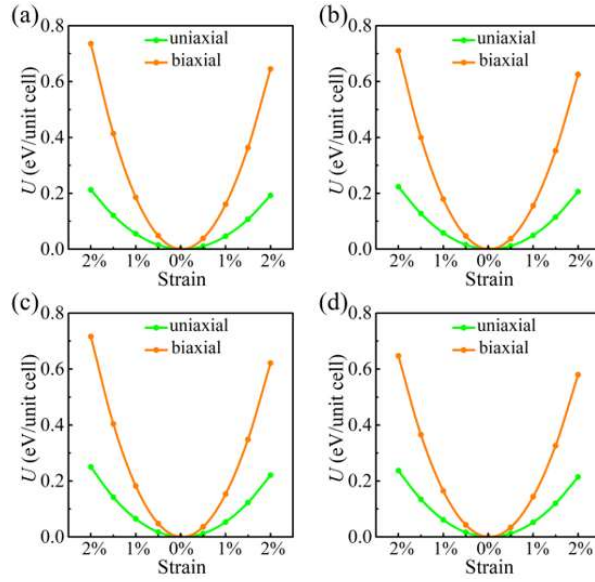
<sup>⊥</sup>Dipartimento di Fisica and INFN, Università di Roma "Tor Vergata", Via della Ricerca Scientifica 1, 00133 Roma, Italy

#### Corresponding Authors

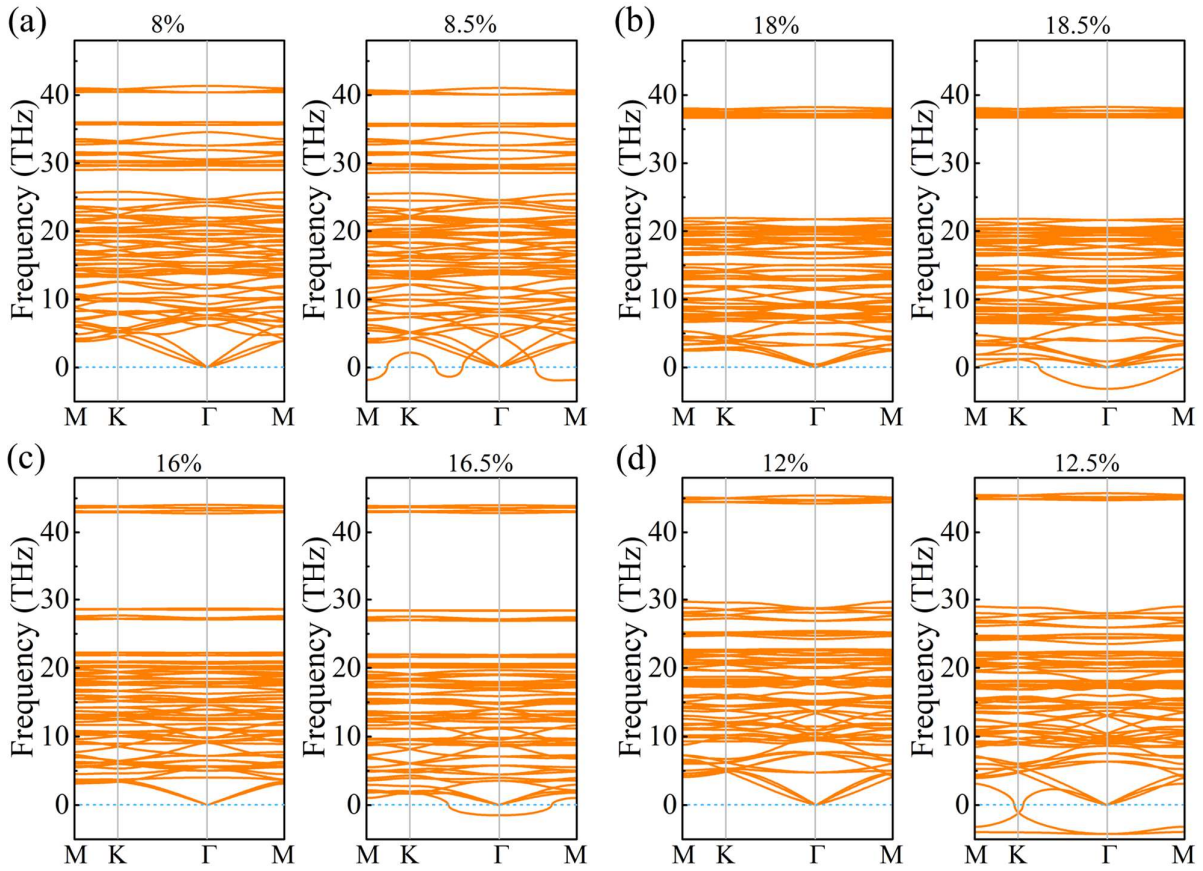
\*W. Zhang (Email: wzhang-1993@stu.xidian.edu.cn)

\*M. Sun (Email: minglei.sun@kaust.edu.sa)

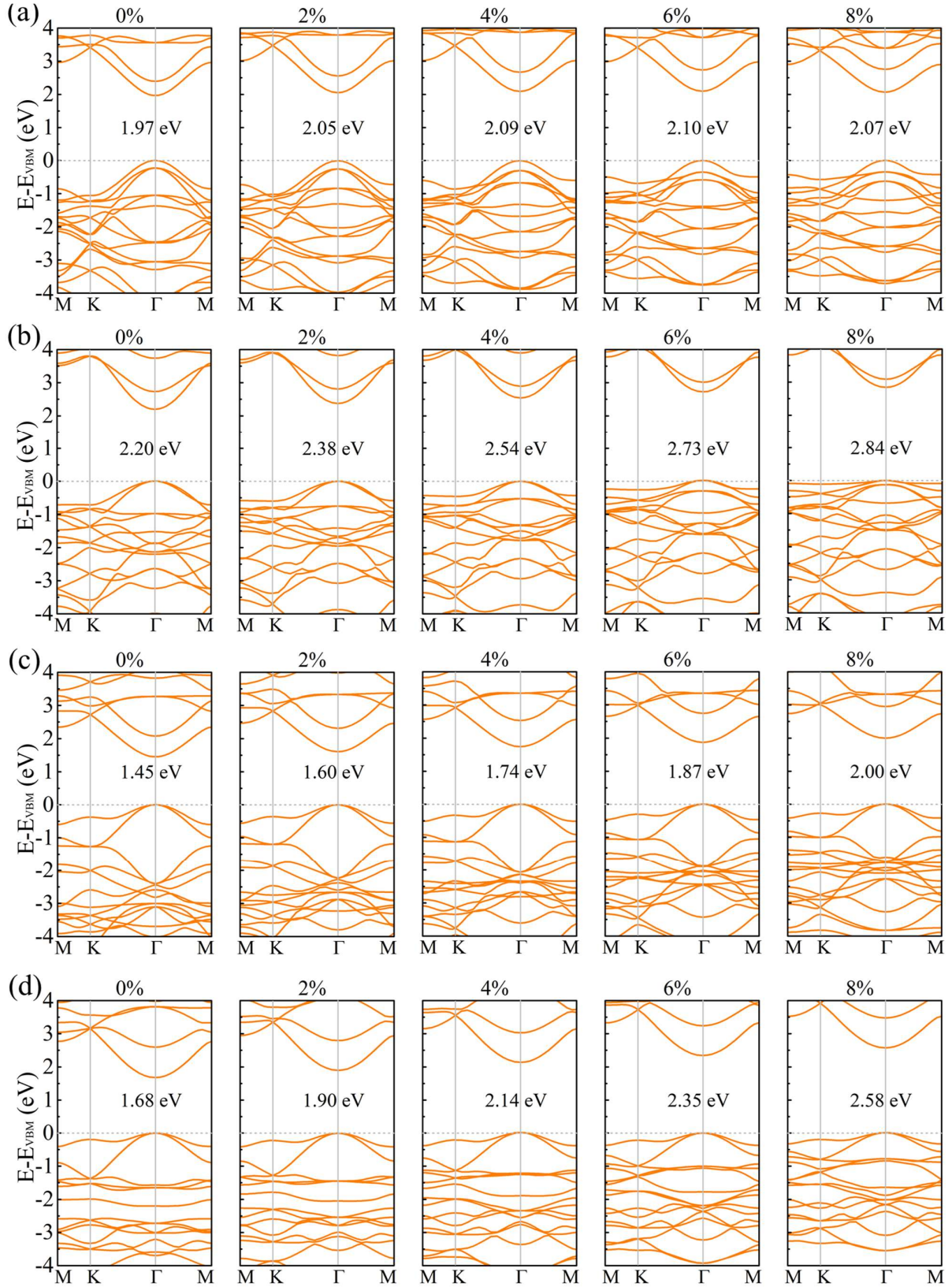
\*U. Schwingenschlöggl (Email: udo.schwingenschlogl@kaust.edu.sa)



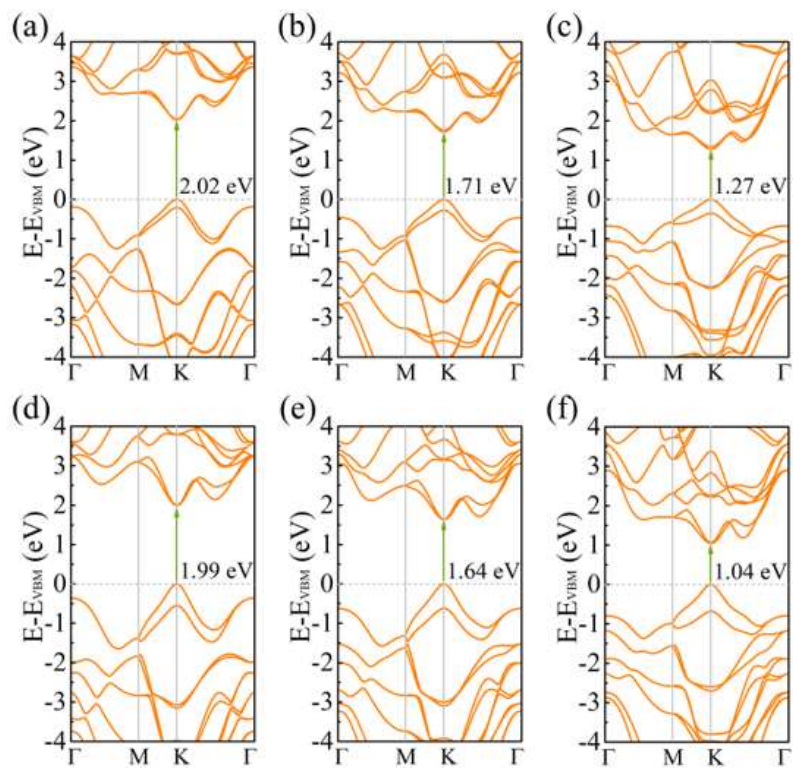
**Figure S1.** Elastic energies of (a)  $\alpha$ -BC<sub>2</sub>N, (b)  $\beta$ -BC<sub>2</sub>N, (c)  $\gamma$ -BC<sub>2</sub>N, and (d)  $\delta$ -BC<sub>2</sub>N under uniaxial and biaxial strain.



**Figure S2.** Phonon spectra of (a)  $\alpha$ -BC<sub>2</sub>N, (b)  $\beta$ -BC<sub>2</sub>N, (c)  $\gamma$ -BC<sub>2</sub>N, and (d)  $\delta$ -BC<sub>2</sub>N under extreme biaxial tensile strain.



**Figure S3.** Electronic band structures of (a)  $\alpha$ -BC<sub>2</sub>N, (b)  $\beta$ -BC<sub>2</sub>N, (c)  $\gamma$ -BC<sub>2</sub>N, and (d)  $\delta$ -BC<sub>2</sub>N under 0%, 2%, 4%, 6%, and 8% biaxial tensile strain.



**Figure S4.** Electronic band structures of 2D (a) MoS<sub>2</sub>, (b) MoSe<sub>2</sub>, (c) MoTe<sub>2</sub>, (d) WS<sub>2</sub>, (e) WSe<sub>2</sub>, and (f) WTe<sub>2</sub> (HSE06+SOC).

POSCAR of  $\alpha$ -BC<sub>2</sub>N

$\alpha$ -BC<sub>2</sub>N

1.0

6.989478111	0.000000000	0.000000000
-3.494739055	6.053065603	0.000000000
0.000000000	0.000000000	25.000000000

N    B    C

6    6    12

Direct

0.200451610	0.400903014	0.536225548
0.599097028	0.799548620	0.536225548
0.200451389	0.799548384	0.536225548
0.799548487	0.599096975	0.536225548
0.400902987	0.200451409	0.536225548
0.799548569	0.200451566	0.536225548
0.202360298	0.404720152	0.594618912
0.595279768	0.797640189	0.594618912
0.202359792	0.797639716	0.594618912
0.797639782	0.595279837	0.594618912
0.404720178	0.202359840	0.594618912
0.797640263	0.202360293	0.594618912
0.000000000	0.400363831	0.517391968
0.599636196	0.599636276	0.517391968
0.400363747	0.000000000	0.517391968
0.000000000	0.599636197	0.517391968
0.400363852	0.400363752	0.517391968
0.599636253	0.000000000	0.517391968
0.000000000	0.402411932	0.618688507
0.597588110	0.597588609	0.618688507
0.402411434	0.000000000	0.618688507
0.000000000	0.597588018	0.618688507
0.402411993	0.402411459	0.618688507
0.597588566	0.000000000	0.618688507

POSCAR of  $\beta$ -BC<sub>2</sub>N

$\beta$ -BC<sub>2</sub>N

1.0

7.054887694	0.000000000	0.000000000
-3.527443846	6.109711964	0.000000000
0.000000000	0.000000000	25.000000000

C    N    B

12    6    6

Direct

0.018200077	0.412200738	0.449806955
0.981799937	0.587799289	0.550193044
0.587799259	0.605999385	0.449806955
0.412200723	0.394000682	0.550193044
0.394000697	0.981800010	0.449806955
0.605999337	0.018200059	0.550193044
0.412200870	0.018200141	0.550193042
0.587799130	0.981799928	0.449806957
0.605999319	0.587799140	0.550193042
0.394000746	0.412200887	0.449806957
0.981799893	0.394000749	0.550193042
0.018200140	0.605999318	0.449806957
0.202661353	0.405322497	0.473711820
0.797338627	0.594677530	0.526288141
0.594677547	0.797338858	0.473711820
0.405322490	0.202661151	0.526288141
0.202661158	0.797338662	0.473711820
0.797338828	0.202661346	0.526288141
0.799289065	0.598578247	0.468711812
0.200710982	0.401421781	0.531288187
0.401421766	0.200710790	0.468711812
0.598578204	0.799289219	0.531288187
0.799289251	0.200710990	0.468711812
0.200710806	0.799289057	0.531288187

POSCAR of  $\gamma$ -BC<sub>2</sub>N

$\gamma$ -BC<sub>2</sub>N

1.0

7.144219796	0.000000000	0.000000000
-3.572109898	6.187075833	0.000000000
0.000000000	0.000000000	25.000000000

C    N    B

12    6    6

Direct

0.1897268517	0.4030883008	0.4728334678
0.5969117101	0.7866385628	0.4728334678
0.2133614361	0.8102731302	0.4728334678
0.1897268517	0.4030883008	0.5271664941
0.5969117101	0.7866385628	0.5271664941
0.2133614361	0.8102731302	0.5271664941
0.4030882778	0.1897268477	0.5271664941
0.7866385758	0.5969117161	0.5271664941
0.8102731122	0.2133614341	0.5271664941
0.4030882778	0.1897268477	0.4728334678
0.7866385758	0.5969117161	0.4728334678
0.8102731122	0.2133614341	0.4728334678
0.0000000000	0.3974533515	0.4494715094
0.6025466714	0.6025466654	0.4494715094
0.3974533225	0.0000000000	0.4494715094
0.0000000000	0.3974533515	0.5505284905
0.6025466714	0.6025466654	0.5505284905
0.3974533225	0.0000000000	0.5505284905
1.0000000000	0.5990671852	0.4525630865
0.4009328377	0.4009328307	0.4525630865
0.5990671892	0.0000000000	0.4525630865
1.0000000000	0.5990671852	0.5474368754
0.4009328377	0.4009328307	0.5474368754
0.5990671892	0.0000000000	0.5474368754

POSCAR of  $\delta$ -BC<sub>2</sub>N

$\delta$ -BC<sub>2</sub>N

1.0

7.132013922	0.000000000	0.000000000
-3.566006960	6.176505236	0.000000000
0.000000000	0.000000000	25.000000000

C    B    N

12    6    6

Direct

0.207170098	0.402836743	0.472834329
0.792829874	0.597163235	0.527165670
0.597163215	0.804333364	0.472834329
0.402836717	0.195666634	0.527165670
0.195666632	0.792829850	0.472834329
0.804333354	0.207170090	0.527165670
0.597163202	0.792829850	0.527165670
0.402836734	0.207170090	0.472834329
0.195666645	0.402836743	0.527165670
0.804333360	0.597163235	0.472834329
0.207170098	0.804333364	0.527165670
0.792829883	0.195666634	0.472834329
1.000000000	0.406384919	0.451175467
1.000000000	0.593615060	0.548824532
0.593615083	0.593615060	0.451175467
0.406384922	0.406384919	0.548824532
0.406384926	0.000000000	0.451175467
0.593615107	0.000000000	0.548824532
1.000000000	0.608820702	0.450691717
1.000000000	0.391179277	0.549308282
0.391179290	0.391179277	0.450691717
0.608820715	0.608820702	0.549308282
0.608820729	0.000000000	0.450691717
0.391179304	0.000000000	0.549308282