Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Oxidation of Two-dimensional Hexagonal Boron Nitride Monolayer: a First-principles Study

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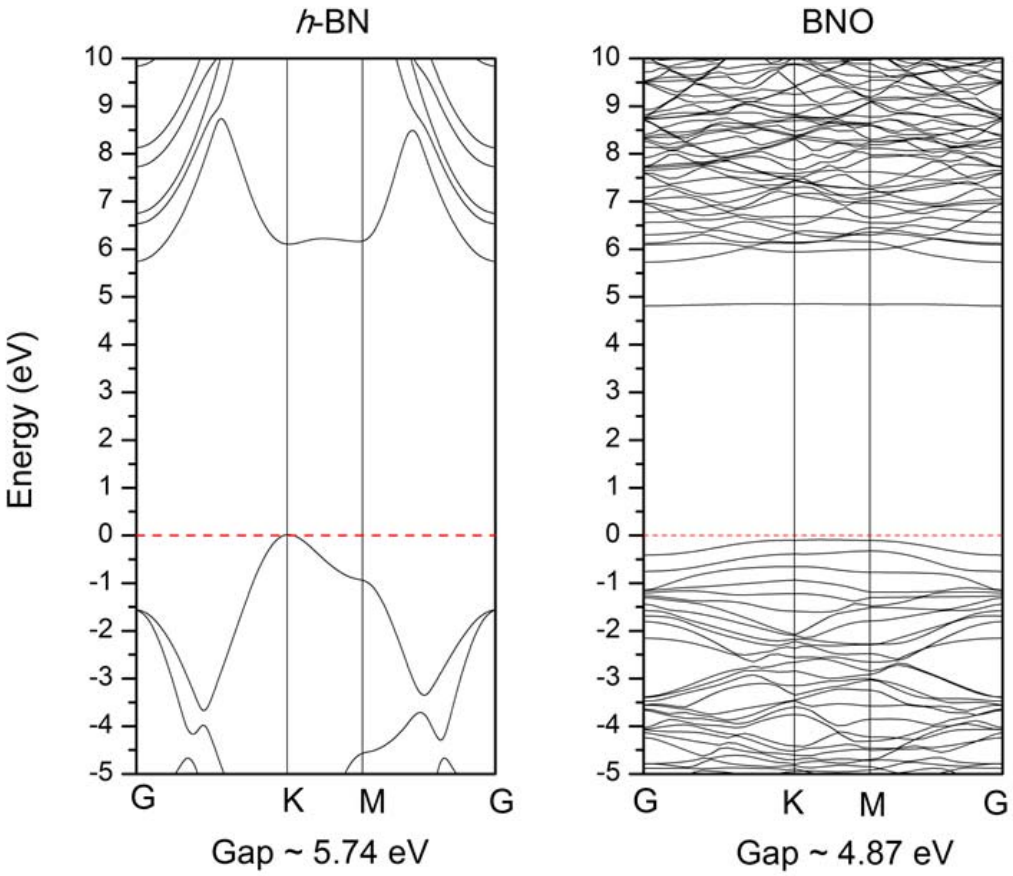

Figure S1: Calculated band structure of pristine *h*-BN sheet and *h*-BNO (i.e. chemisorption of atomic O per supercell on the *h*-BN sheet), by using the HSE06 hybrid functional implemented in the VASP package.

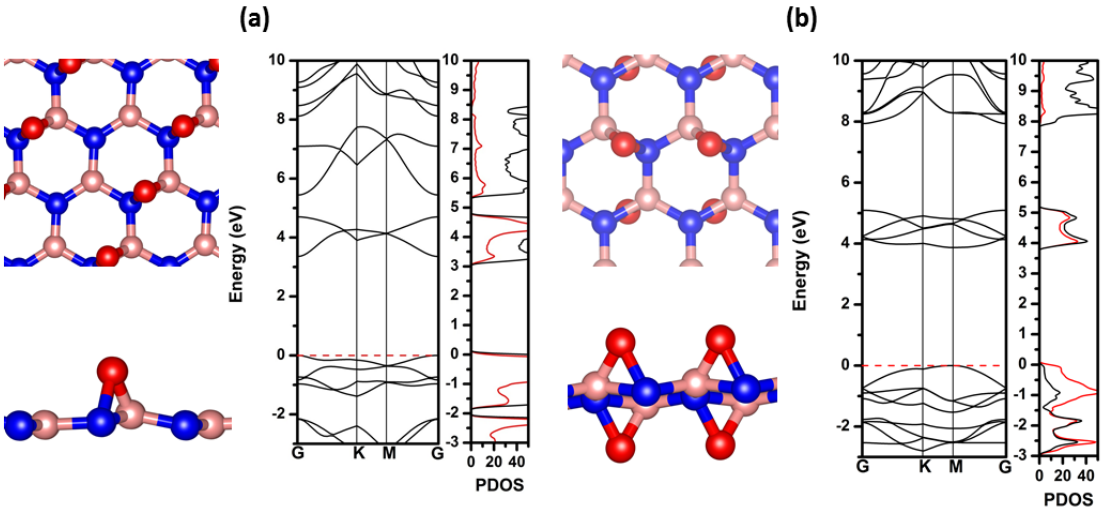

Figure S2: Top and side view of optimized structures of *h*-BN oxide with (a) 50% and (b) 100% atomic O coverage. The calculated band structures (PBE) and PDOS are shown in the right panel. The DOS projected on a single O atom and a B-N pair is plotted with red solid line and black solid line, respectively. The red dashed line denotes the Fermi level. Red, blue, pink spheres represent O, N, B, respectively.

Table S1: Relative energies per supercell (ΔE), adsorption energies of a single atomic O (E_{ads}), B-N bond length (in the BNO ring, L_{BN}), band gap (E_g) of *h*-BN sheet with two chemisorbed O atoms (per supercell) either on single side (*ss*) or on both side (*bs*). (a) – (d) refer to chemisorption configurations shown in **Figure 2a-2d**.

	ΔE (eV)	E_{ads} (eV)	L_{BN} (Å)	E_g (eV)
bs-BN-O2 (a)	0	2.34	1.54	3.29
bs-BN-O2 (c)	0.02	2.33	1.57, 1.58	3.16
ss-BN-O2 (a)	0.11	2.29	1.59, 1.61	3.37
ss-BN-O2 (b)	0.14	2.27	2.18	4.22
ss-BN-O2 (c)	0.20	2.24	1.57, 1.59	3.07
bs-BN-O2 (d)	0.46	2.11	1.60	2.99
ss-BN-O2 (d)	0.51	2.09	1.60,1.61	2.97
bs-BN-O2 (b)	0.64	2.02	1.59	2.64