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

Supporting Information

Enhanced Selective Oxidation of h-BN Nanosheet through Substrate Mediated Localized Charge Effect

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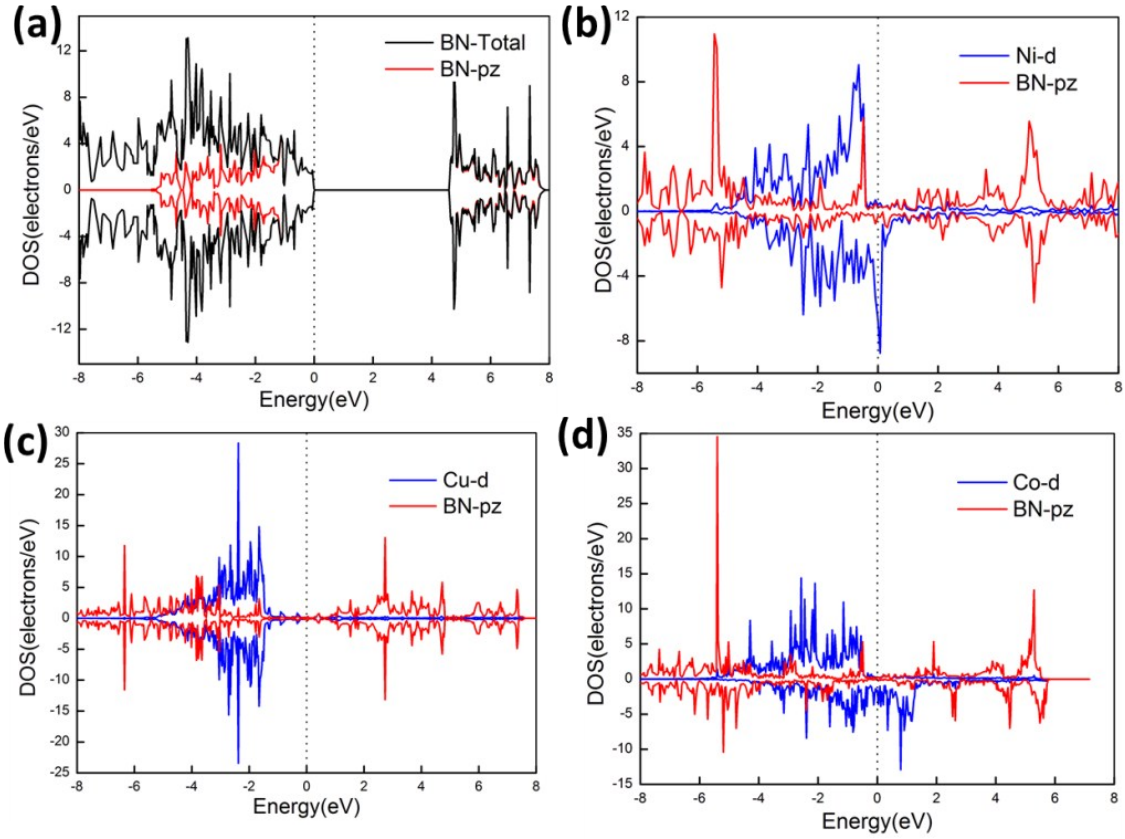

Figure S1 The density of states (DOS) of (a) pure h-BN monolayer, (b) *h*-BN/Ni(111), (c) *h*-BN/Cu(111), and (d) *h*-BN/Co(001) projected on p_z orbitals of B and N, and *d* orbitals of metals are plotted. The Fermi energy level is set as zero.

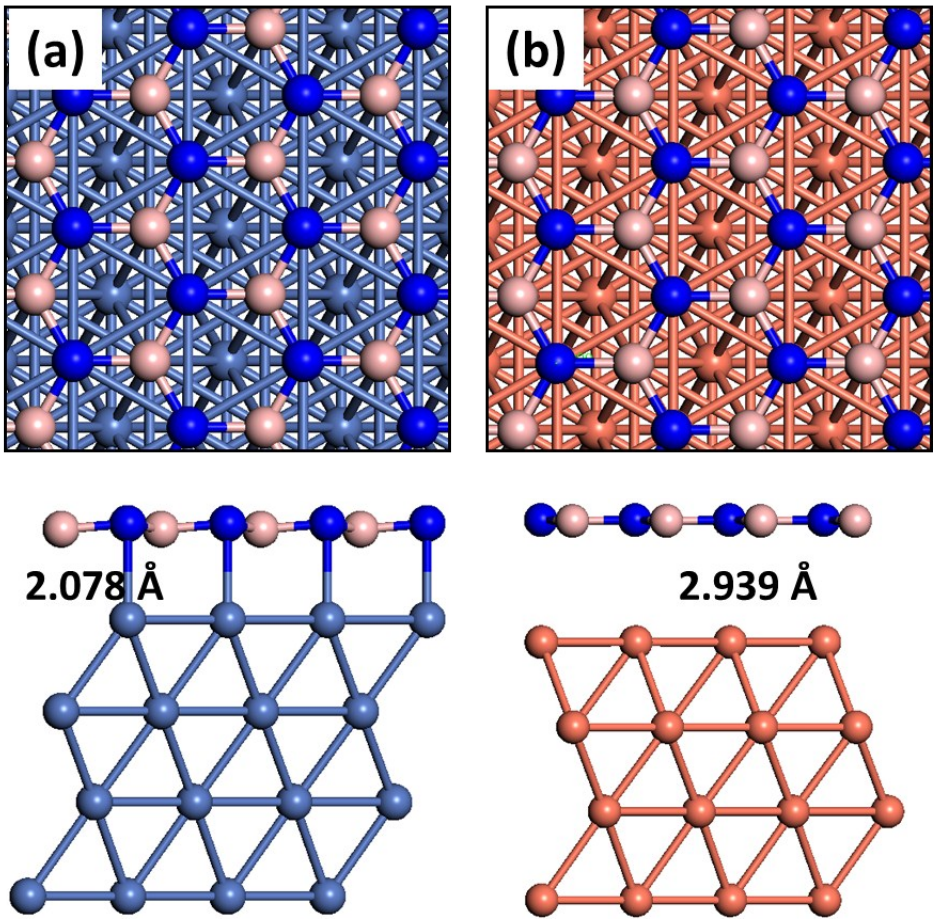

Figure S2 Top and side views of the optimized structures of (a) *h*-BN/Ni(111) and (b) *h*-BN/Cu(111) with boron atoms occupying the hcp site of substrate.

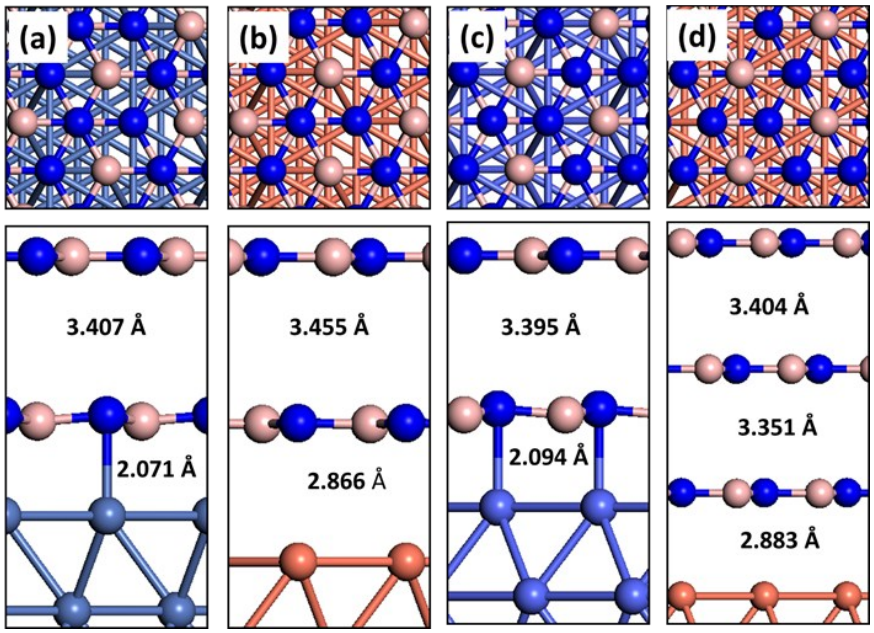

Figure S3 The top and side views of the optimized structures of *h*-BN bilayer on (a) Ni(111), (b) Cu(111), (c)Co(001) substrates, and *h*-BN triple layer on (d) Cu(111) substrate.

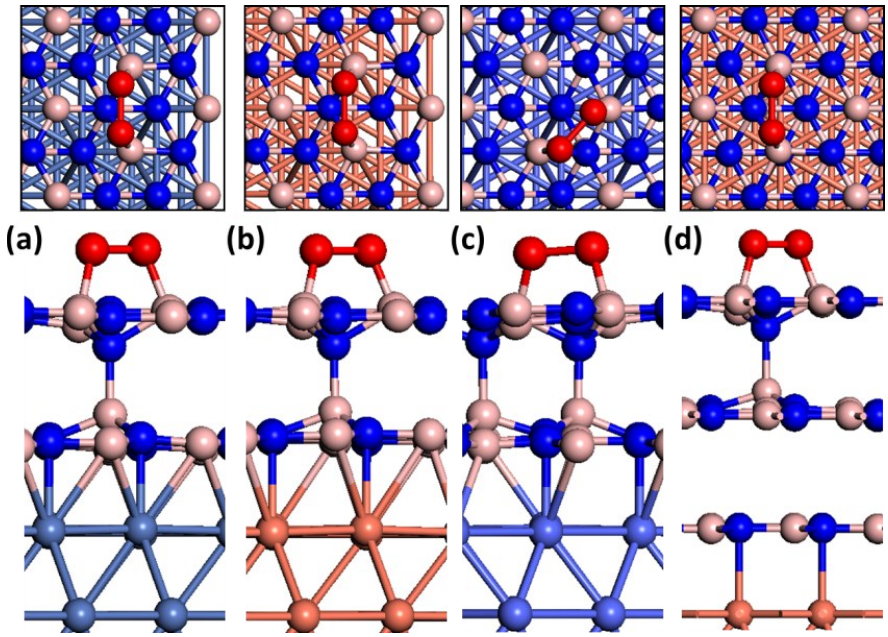

Figure S4. Top and side views of O_2 adsorbed structure on *h*-BN bilayer supported by (a) Ni(111), (b) Cu(111), (c) Co(001), and *h*-BN triple layer supported by (d) Cu(111) substrate.

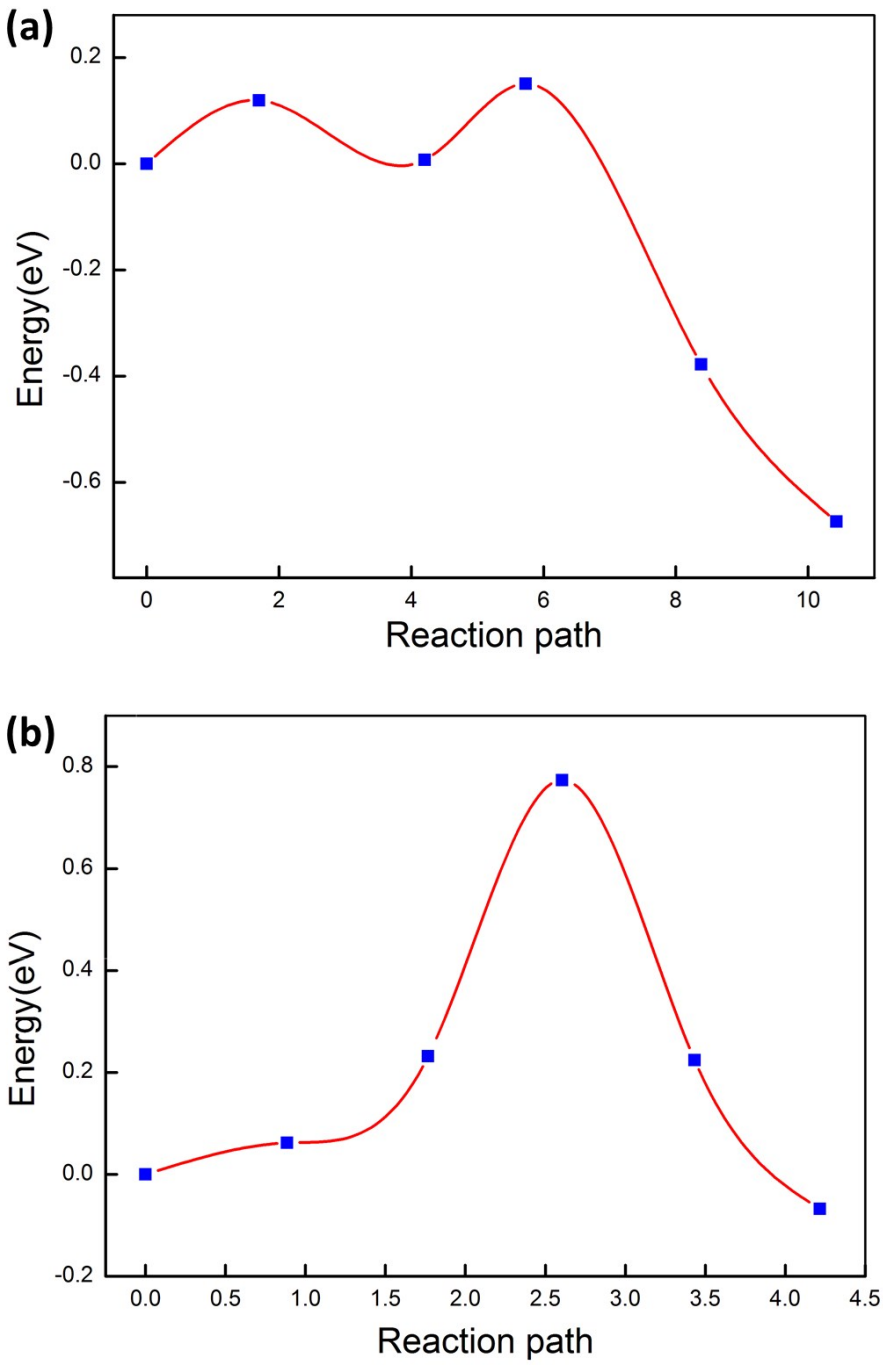

Figure S5. The calculated MEP for O_2 chemisorbed on *h*-BN bilayer supported by (a) Cu(111) and (b) Ni(111) substrates, respectively.

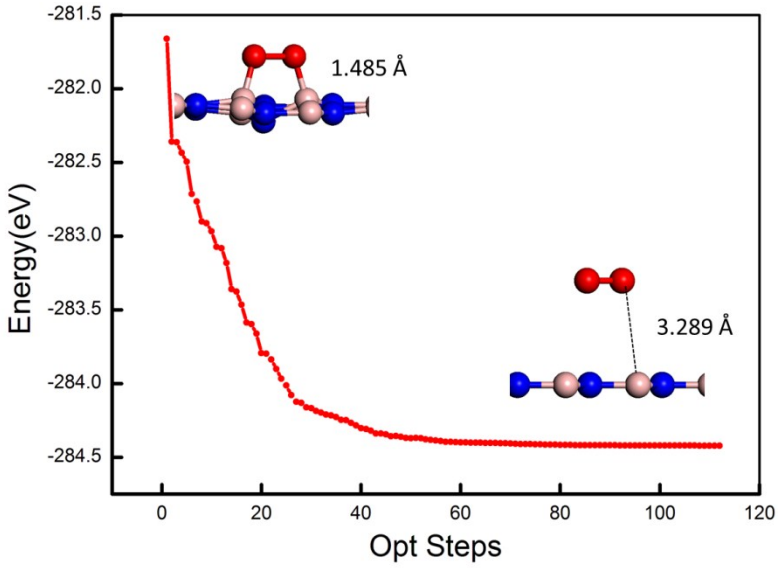

Figure S6. The total energy versus optimization steps for O_2 molecule on freestanding *h*-BN monolayer with 2.5% biaxial strain. The initial structure is taken from the O_2 adsorbed structure on h-BN/Cu(111) species

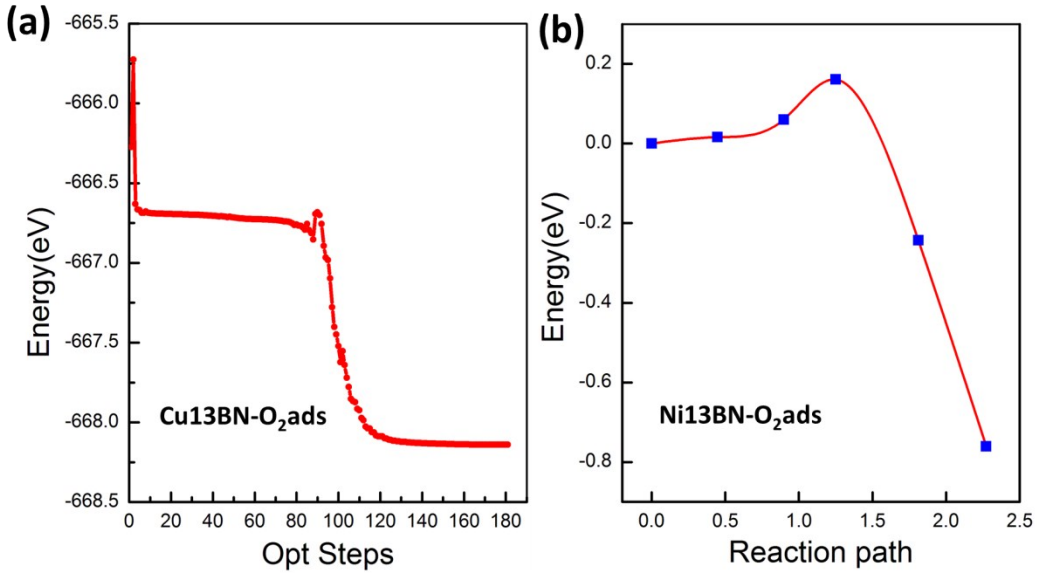

Figure S7. (a) The energy profile versus optimization step for O_2 adsorption on *h*-BN/Cu_{13}, indicating that the adsorption process is spontaneous. (b) The calculated MEP for the O_2 adsorption on *h*-BN/Ni_{13}.

TABLE S1 The adsorption energy (E_{ads}), local magnetic moment on O atom (M), the O-O bond lengths ($d_{O\text{-}O}$), and charge transfer from *h*-BN sheet to O_2 specie (C) are summarized for *bi-h*-BN/Cu(111), *bi-h*-BN/Ni(111), *bi-h*-BN/Co(001), and *tri-h*-BN/Cu(111).

	O_2/*bi-h*-BN/Ni(111)	O_2/*bi-h*-BN/Cu(111)	O_2/*bi-h*-BN/Co(001)	O_2/*tri-h*-BN/Cu(111)
E_{ads} (eV)	-0.165	-0.757	0.112	0.881
M (μ_B)	0.202 0.202	-0.079 -0.079	-0.047 -0.050	0.285 0.285
$d_{O\text{-}O}$ (Å)	1.401	1.458	1.449	1.388
C (e)	1.186	1.473	1.449	1.057

TABLE S2 The adsorbed O_2 properties on electron doped *h*-BN monolayer. The adsorption energy (E_{ads}) and O-O bond length (L(O-O)) are listed in the below table. "number *e*" indicates the number of electrons per supercell are introduced to *h*-BN monolayer.

	1 *e*	2 *e*	3 *e*
E_{ads} (eV)	-0.972	-1.702	-2.568
$L_{O\text{-}O}$ (Å)	1.343	1.485	1.511

Table S3. The adsorption energy (E_{ads} in unit of eV) and O-O bond lengths ($d_{O\text{-}O}$ in unit of Å) for O_2 molecule adsorbed on Ni_{13} and Cu_{13} supported *h*-BN monolayer.

	Cu_{13}				Ni_{13}			
	C1	E1	E2	F1	C1	E1	E2	F1
E_{ads}	-2.028	-1.514	-1.961	-0.408	-0.886	-0.418	-0.108	01.36
$d_{O\text{-}O}$	1.441	1.414	1.441	1.266	1.427	1.404	1.327	1.242