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

Supplementary data to:

Theoretical study on the origin of activity for oxygen reduction reaction of metal doped two-dimensional boron nitride materials

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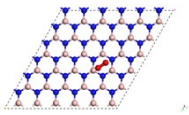
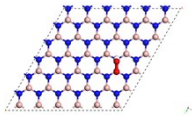
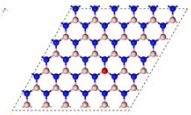
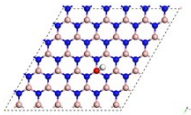
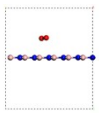
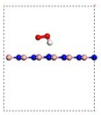
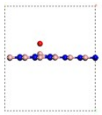
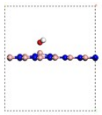
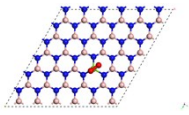
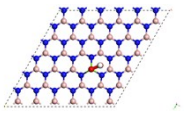
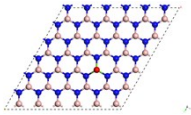
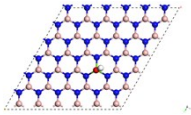
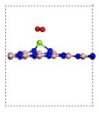
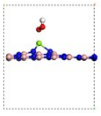
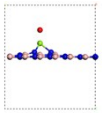
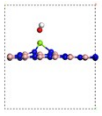
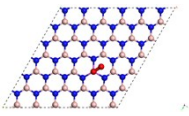
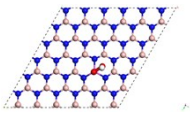
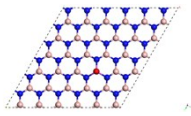
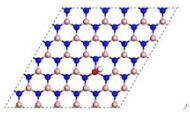
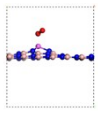
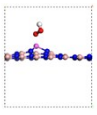
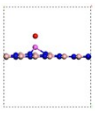
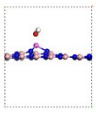
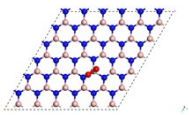
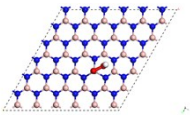
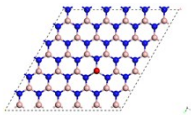
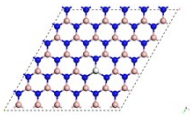
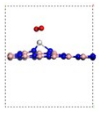
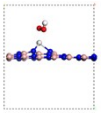
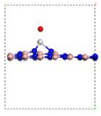
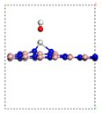
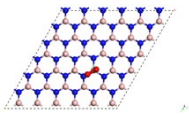
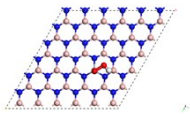
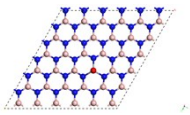
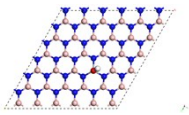
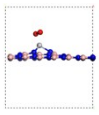
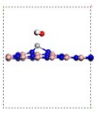
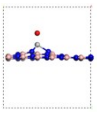
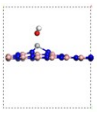
Content

Table S1. Optimized adsorption configurations (top and side views) of key oxygenated intermediates involved in the ORR on M–BN materials (red: oxygen atoms; white: hydrogen atoms; blue: nitrogen atoms).

Catalysts	*O2	*OOH	*O	*OH
BN				
BN				
Mg–BN				
Mg–BN				
Al–BN				
Al–BN				
Sc–BN				
Sc–BN				
Ti–BN				
Ti–BN				
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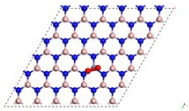
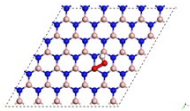
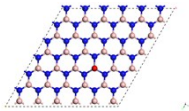
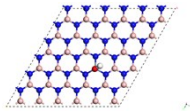
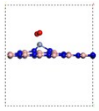
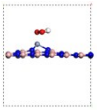
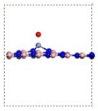
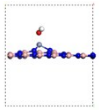
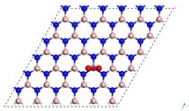
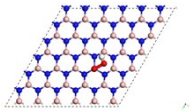
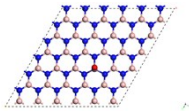
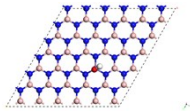
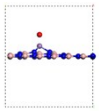
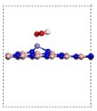
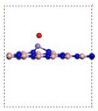
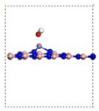
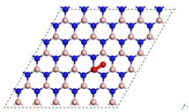
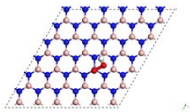
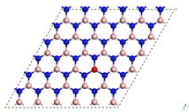
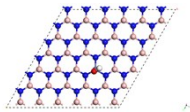
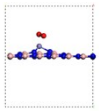
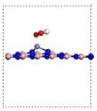
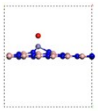
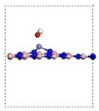
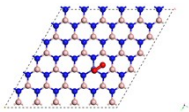
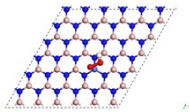
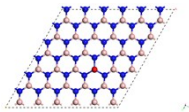
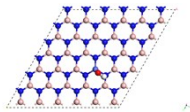
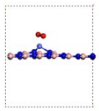
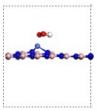
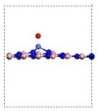
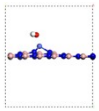
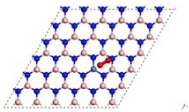
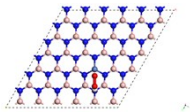
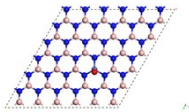
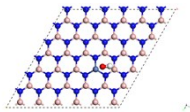
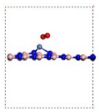
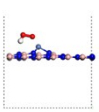
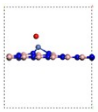
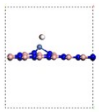
V–BN				

Cr–BN				
Cr–BN				
Mn–BN				
Mn–BN				
Fe–BN				
Fe–BN				
Co–BN				
Co–BN				
Ni–BN				
Ni–BN				
Cu–BN				
Cu–BN				
Zn–BN				
Zn–BN				

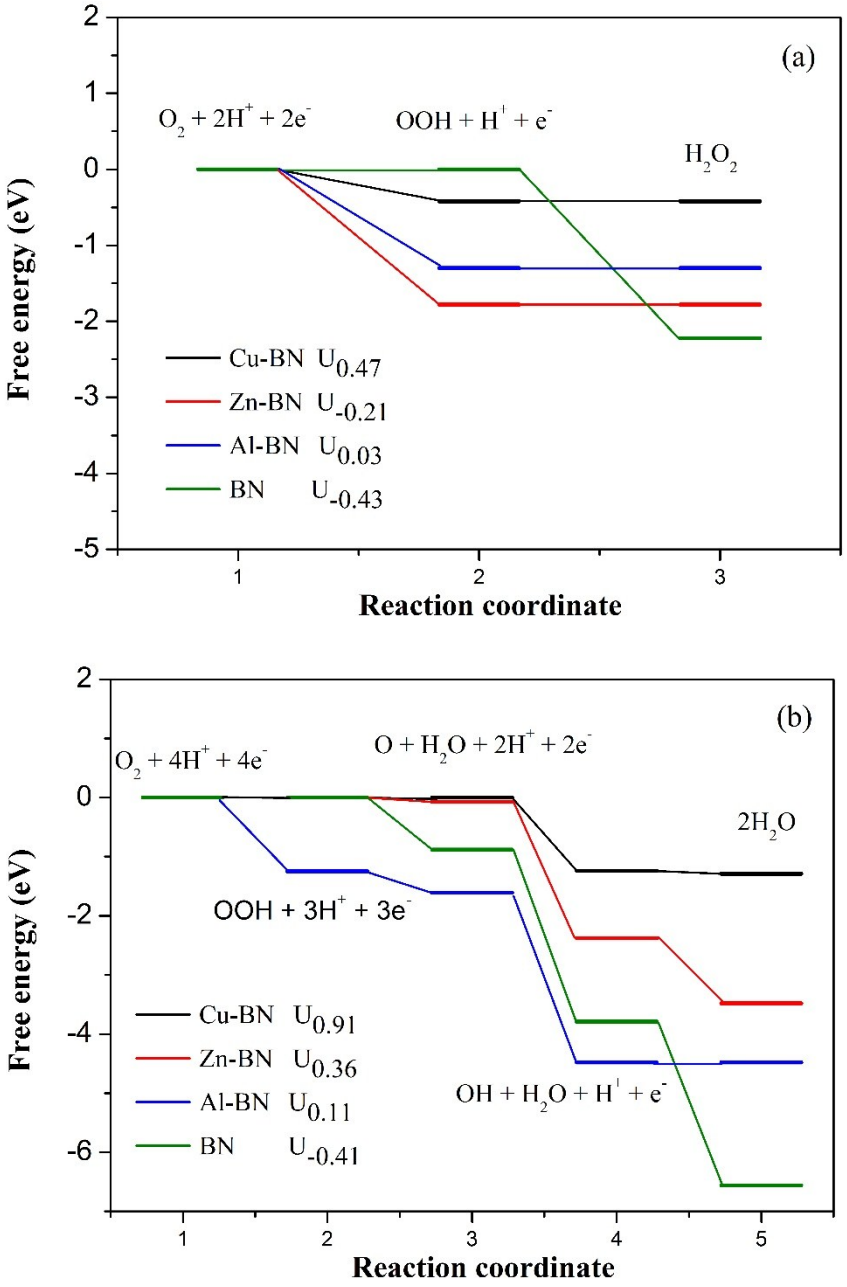
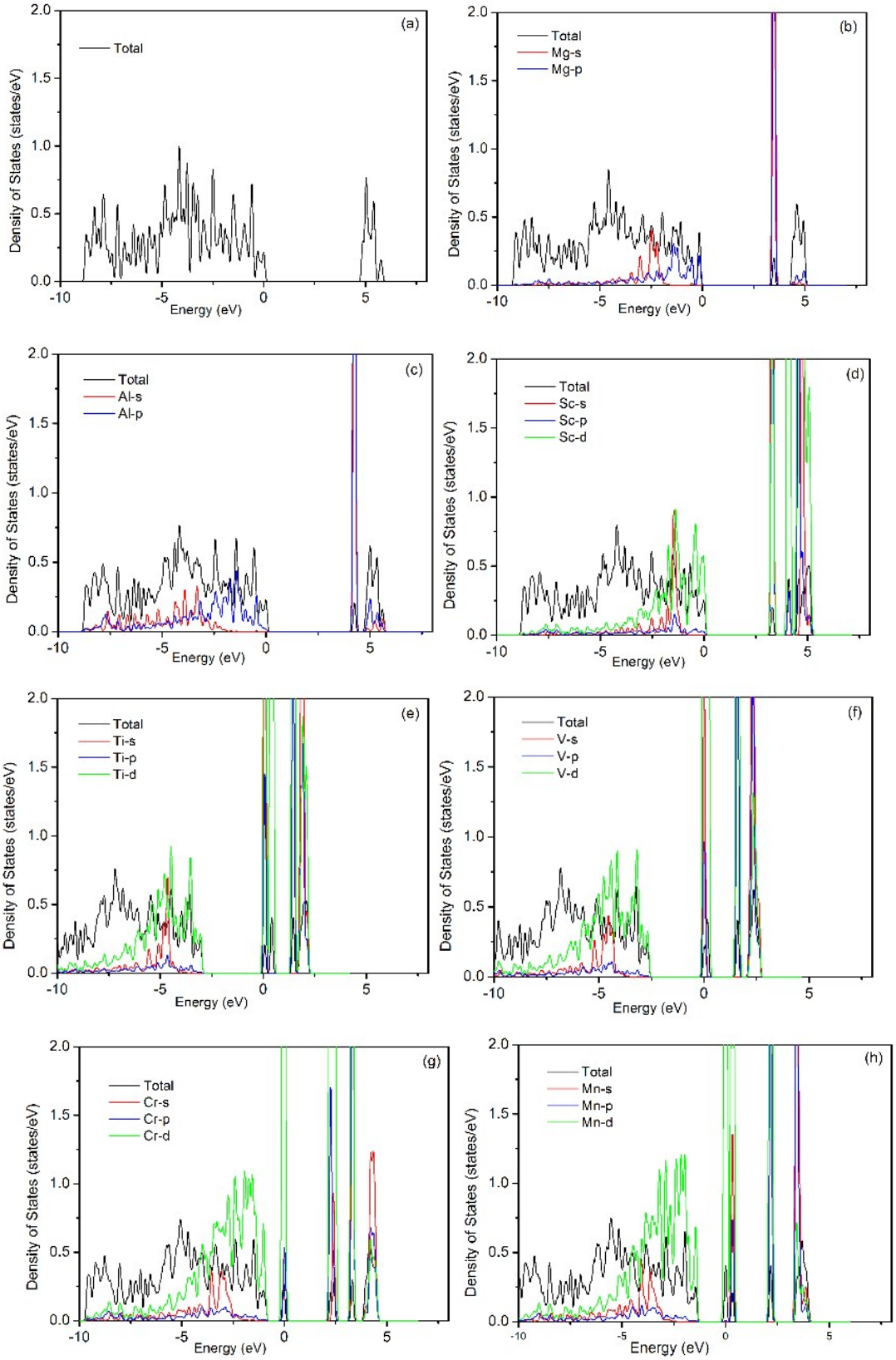


Figure S1. The free energy diagram at the onset potentials for Cu–BN, Zn–BN, Al–BN and BN materials (a) the $2e^-$ mechanism, (b) the $4e^-$ mechanism.


(a)
Total
(b)
Total
Mg-s
Mg-p
(c)
Total
Al-s
Al-p
(d)
Total
Sc-s
Sc-p
Sc-d
(e)
Total
Ti-s
Ti-p
Ti-d
(f)
Total
V-s
V-p
V-d
(g)
Total
Cr-s
Cr-p
Cr-d
(h)
Total
Mn-s
Mn-p
Mn-d
Density of States (states/eV)
Energy (eV)

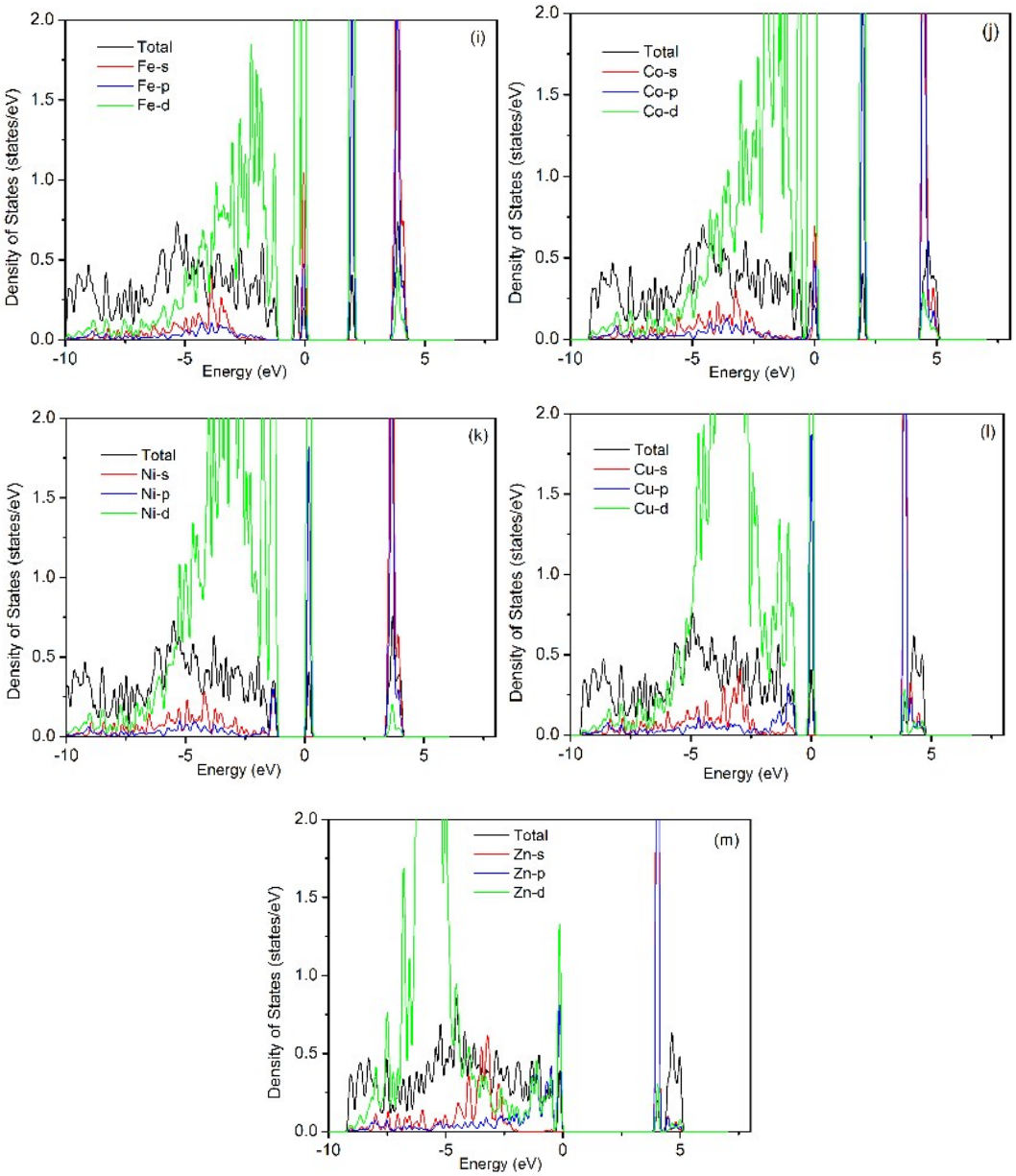
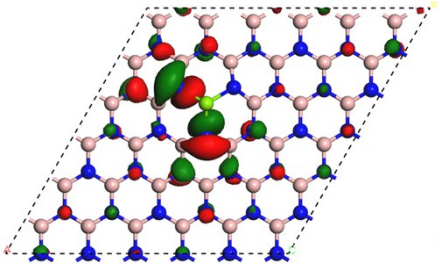
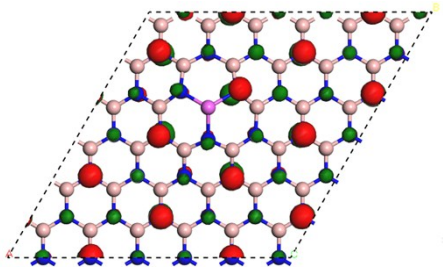


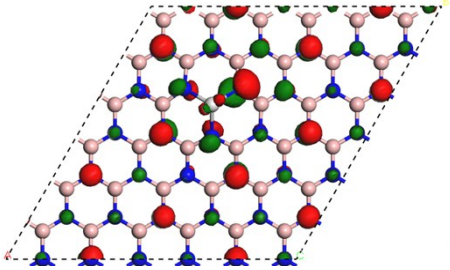
Figure S2. The local density of states for M–BN materials (a) pristine state of BN,(b) Mg–BN, (c) Al–BN, (d) Sc–BN, (e) Ti–BN, (f) V–BN, (g) Cr–BN,(h) Mn–BN, (i) Fe–BN, (j) Co–BN, (k) Ni–BN, (l) Cu–BN, (m) Zn–BN.



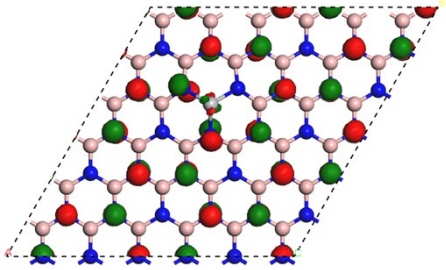
(a) Mg–BN



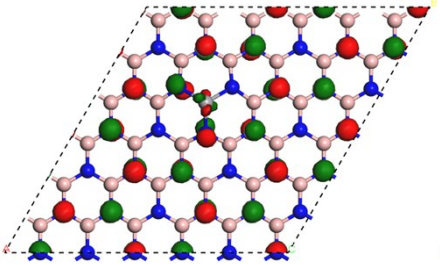
(b) Al–BN



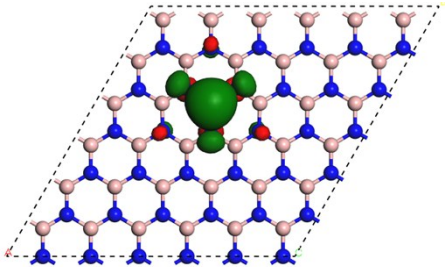
(c) Sc–BN



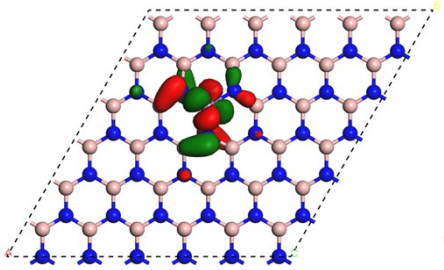
(d) Ti–BN



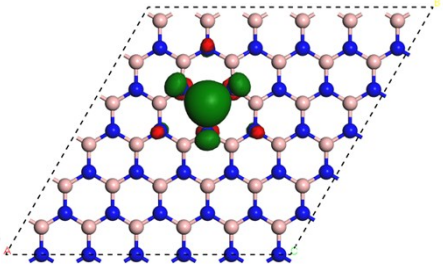
(e) V–BN



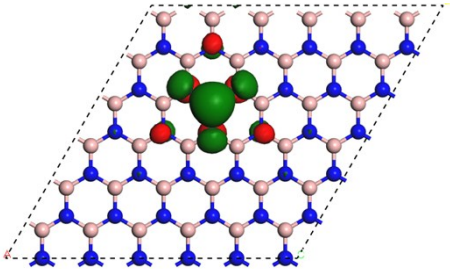
(f) Cr–BN



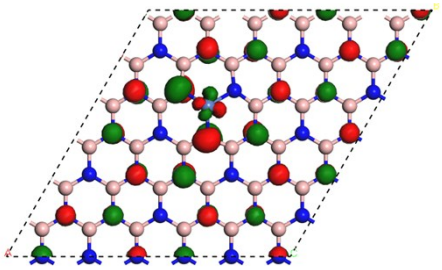
(g) Mn–BN



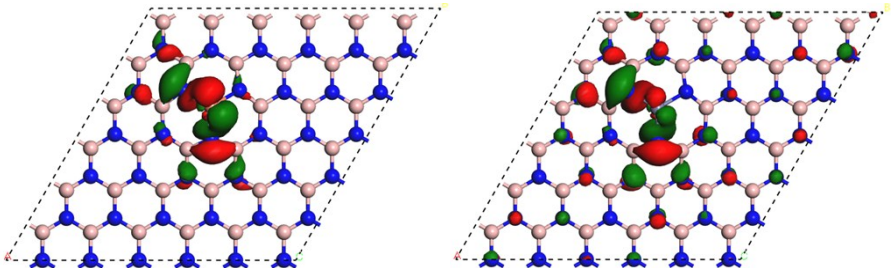
(h) Fe–BN



(i) Co–BN



(j) Ni–BN



(k) Cu–BN (l) Zn–BN

Figure S3. The highest occupied molecular orbital (HOMO) of (a) Mg–BN, (b) Al–BN, (c) Sc–BN, (d) Ti–BN, (e) V–BN, (f) Cr–BN, (g) Mn–BN, (h) Fe–BN, (i) Co–BN, (j) Ni–BN, (k) Cu–BN, (l) Zn–BN

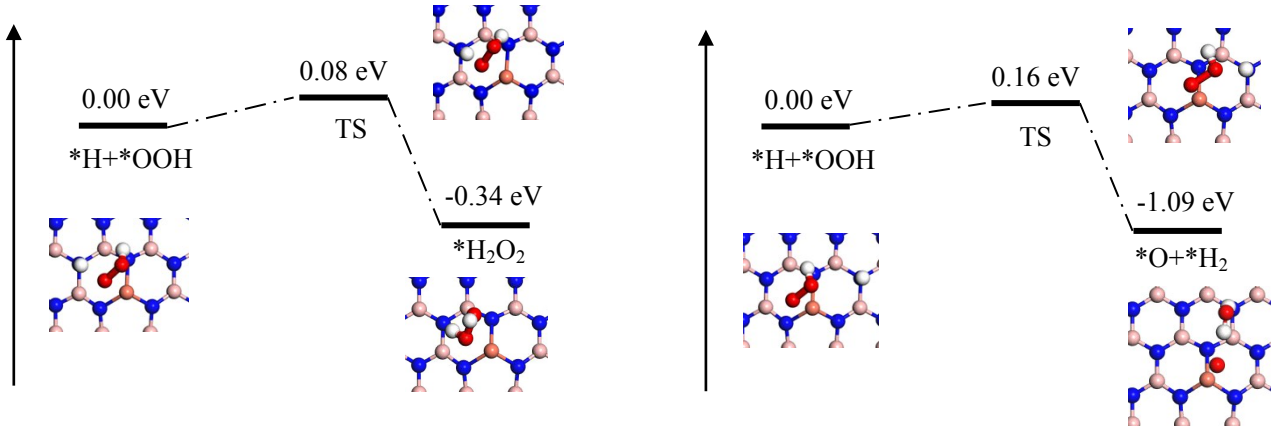


Figure S4. The pathways of the 2e⁻ mechanism for Cu–BN materials.

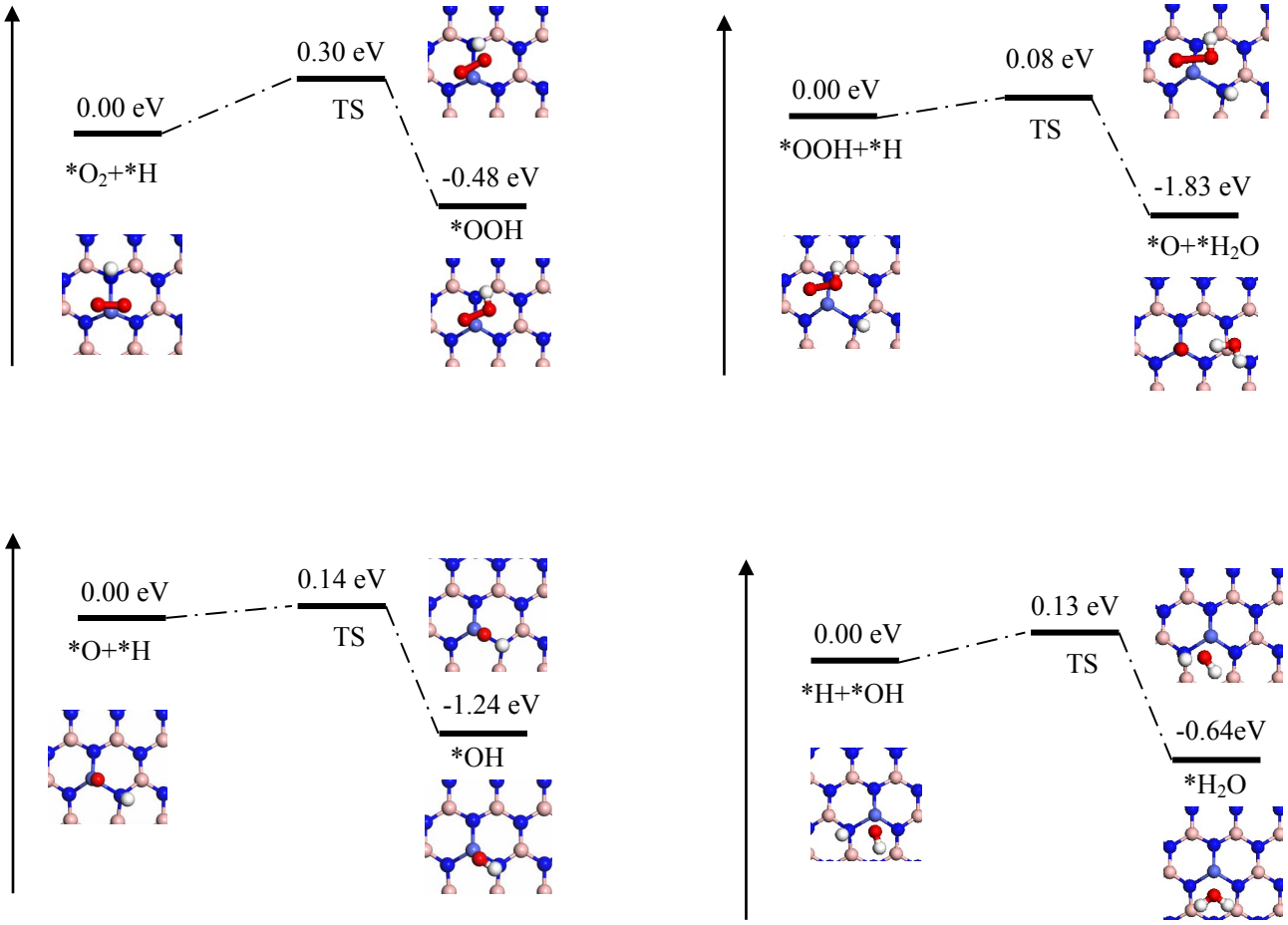


Figure S5. The pathways of the 4e⁻ mechanism for Co–BN materials.