Supporting Information

The role of potassium in activation of oxygen to promote nitric oxide oxidation on honeycomb-like h-BN (001) surface

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1. *k*-point convergence test

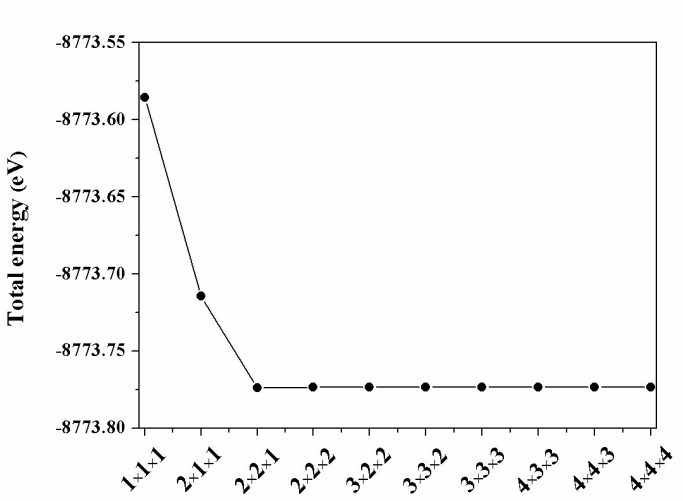

Fig. S1 The *k*-point convergence test of h-BN (001) surface.

2. Surface energy convergence test

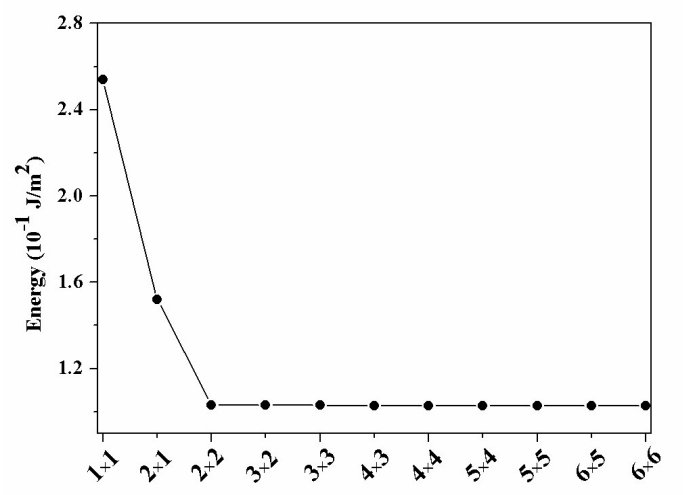

Fig. S2 The surface energy of h-BN (001) surface.

3. The relaxed configurations of K-BN

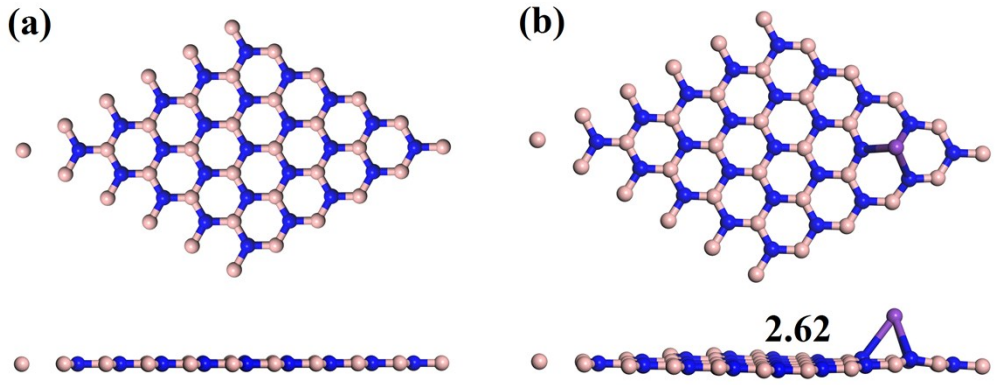

Fig. S3 The relaxed configurations of pure (a) and K-doped (b) h-BN (001) surfaces. (Lengths in Å.)

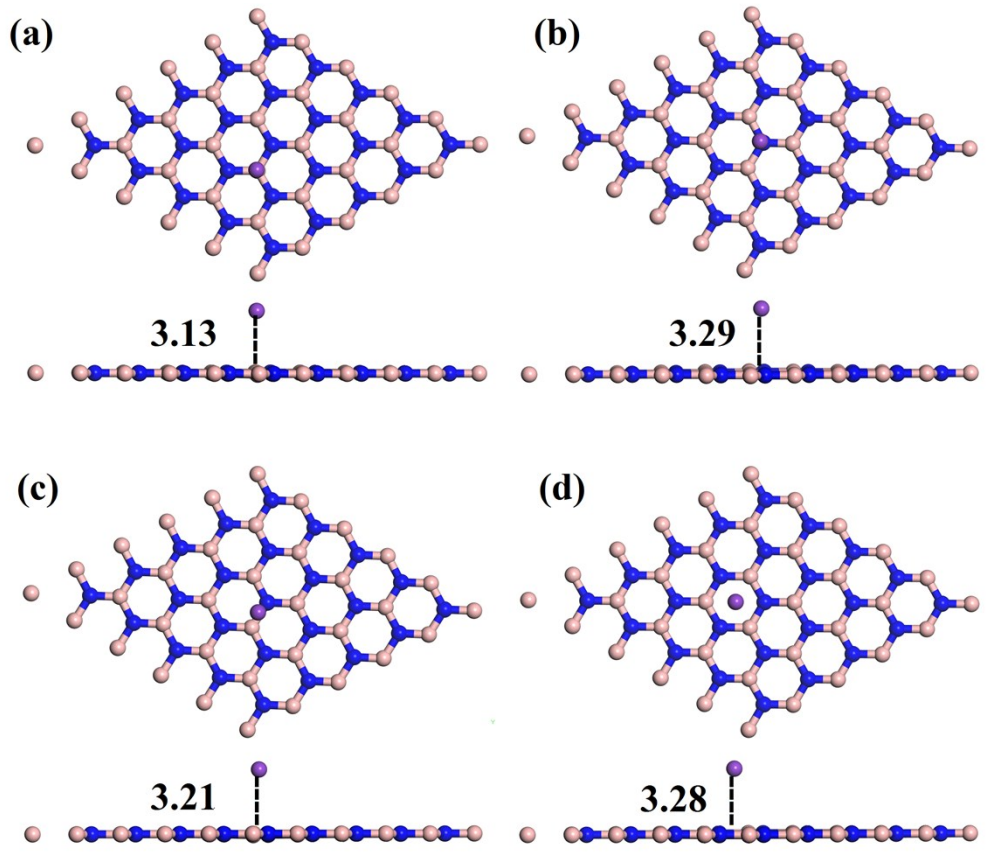

Fig. S4 The relaxed configurations of K loaded at B (a), N (b), bridge of BN bond (c) and hexagon BN ring (d) sites of h-BN (001) surface. (Lengths in Å.)

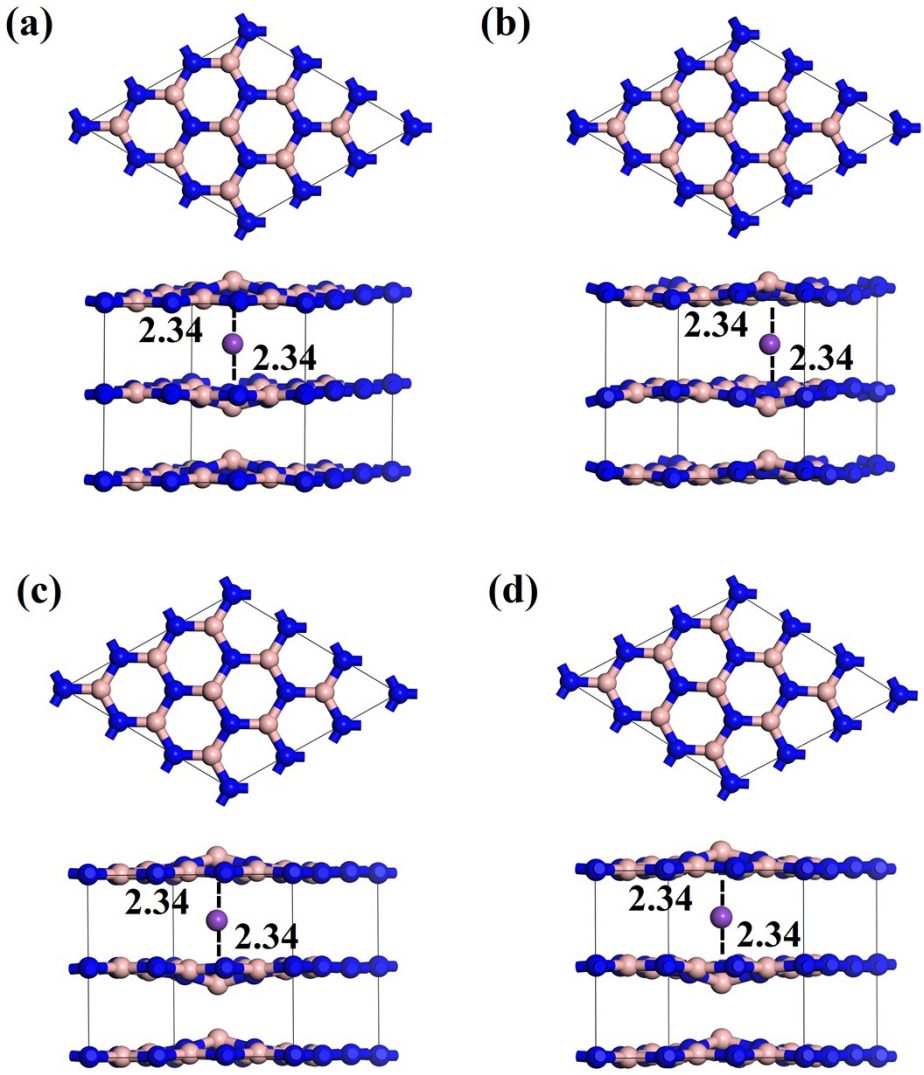

Fig. S5 The relaxed configurations of K intercalated at B (a), N (b), bridge of BN bond (c) and hexagon BN ring (d) sites of h-BN. (Lengths in Å.)

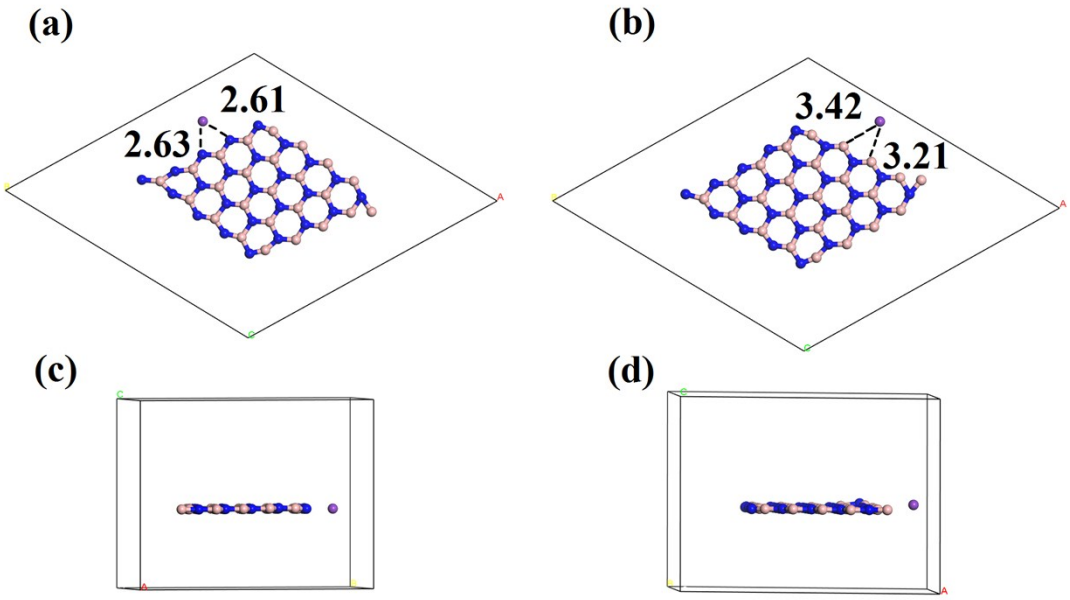

Fig. S6 The relaxed configurations of K doped at N (a) and B-terminated (b) defective edge sites of h-BN. (Lengths in Å.)

4. The adsorption of gas molecule on pure and K-modified h-BN surface

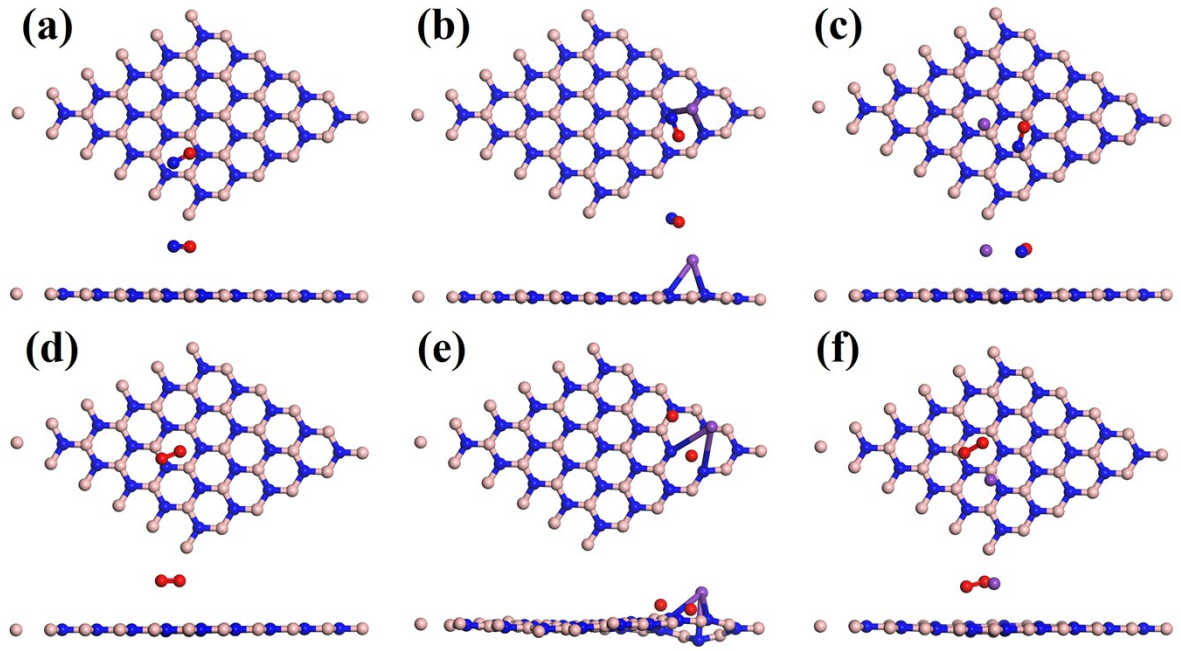

Fig. S7 The adsorption structures of individual NO and O_2 on pure (a, d), K-doped (b, e) and loaded (c, f) h-BN.

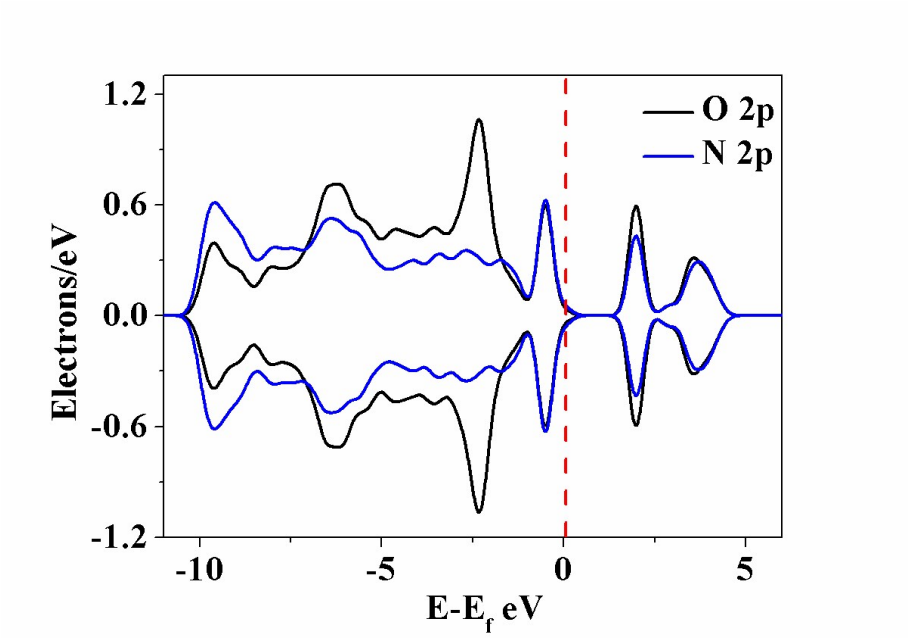

Fig. S8 The PDOS of O_2 adsorbed on K-doped h-BN surface. (The red dotted lines stand for Fermi level.)

5. Configurations of NO oxidation on pure and K-modified h-BN surface

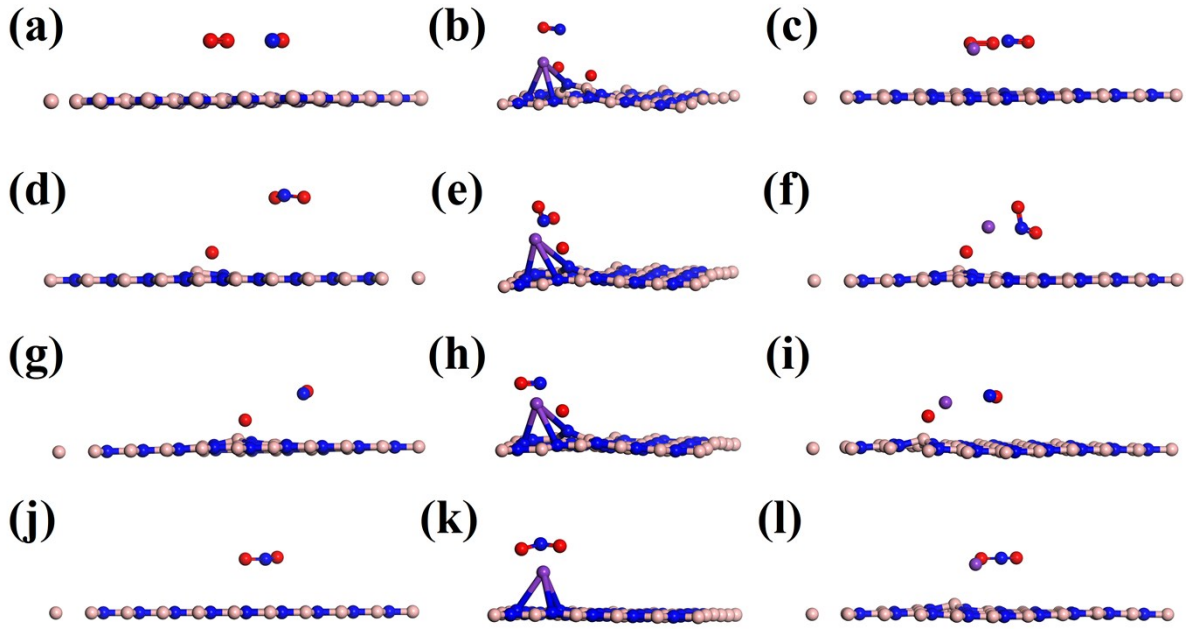

Fig. S9 The structures corresponding to the reaction path followed by the NO oxidation mechanism 1 on pure, (a, d, g, j) K-doped (b, e, h, k) and loaded (c, f, i, l) h-BN surface.

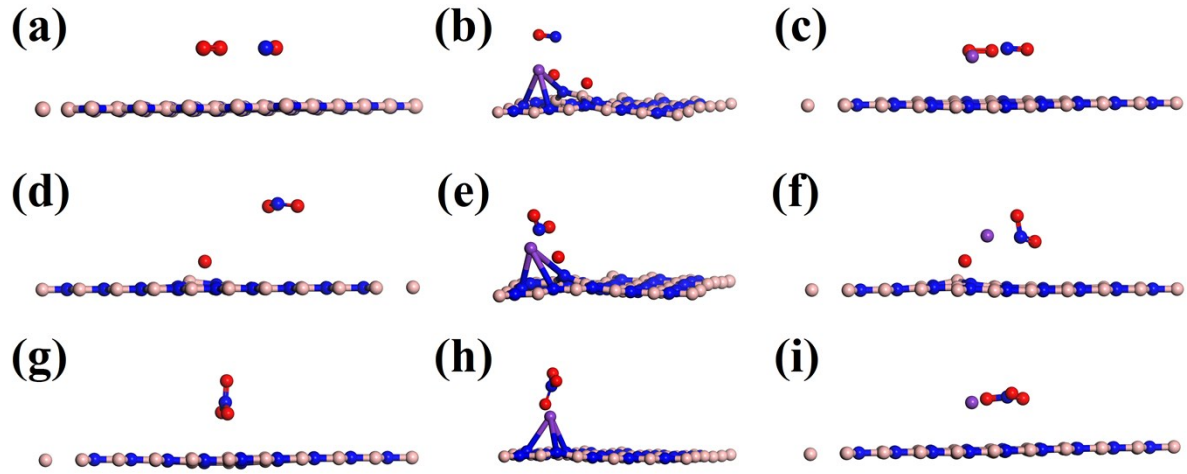

Fig. S10 The structures corresponding to the reaction path followed by the NO oxidation mechanism 2 on pure, (a, d, g, j) K-doped (b, e, h, k) and loaded (c, f, i, l) h-BN surface.

6. The unit parameters of B, K, KN_3 and $B_{5.67}K$ crystals

Table S1 The unit parameters of B and K crystals. (Lengths in Å, angles in °.)

Crystal	Lattice parameters
B	$a=b=4.908$, $c=12.567$
	$\alpha=\beta=90$, $\gamma=120$
K	$a=b=c=13.676$
	$\alpha=\beta=\gamma=90$
KN_3	$a=b=6.094$, $c=7.056$
	$\alpha=\beta=\gamma=90$
$B_{5.67}K$	$a=b=c=4.222$
	$\alpha=\beta=\gamma=90$