Supplementary data to:

Single-atom catalyst of cobalt supported on defective two-dimensional boron nitride material as a promising electrocatalyst for oxygen reduction reaction: A DFT study

Chaofang Deng [a,b,c], Rongxing He[a], Wei Shen[a], Ming Li [a] * and Tao Zhang[b]

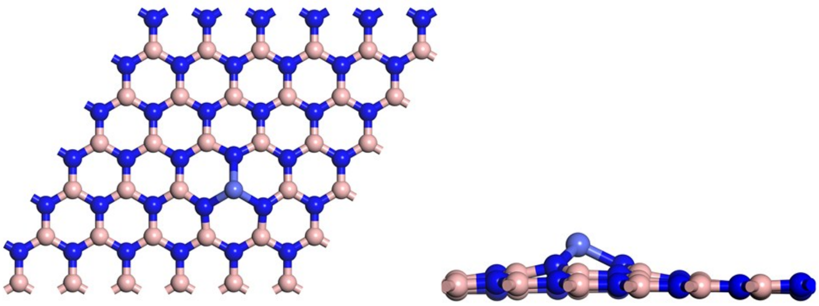
[a]Key Laboratory of Luminescence and Real-Time Analytical Chemistry (Southwest University), Ministry of Education, College of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, China

[b]College of Biological and Chemical Engineering, Chongqing University of Education, Chongqing 400067, China

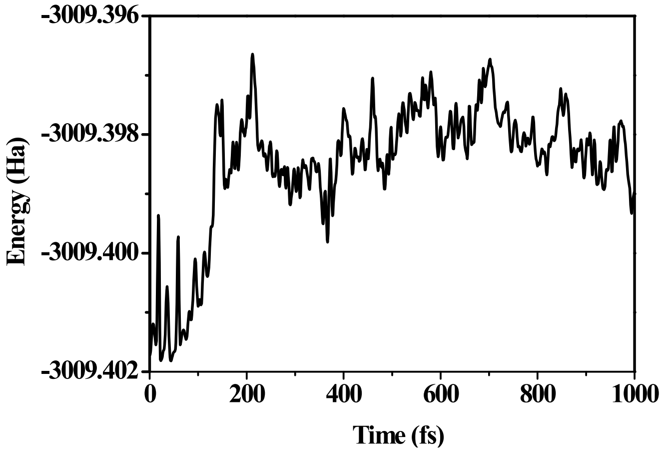
[c]Cooperative Innovation Center of Lipid Resources and Children's Daily Chemicals, Chongqing University of Education, Chongqing 400067, China

* To whom correspondence should be addressed. E-mail: liming@swu.edu.cn

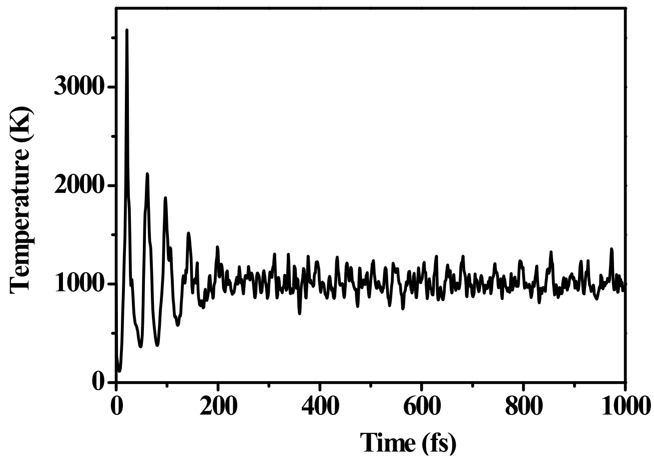
Content



(a)



(b)



(c)

Fig. S1. (a) The atomic structure (b) total energy and (c) temperature of single Co atom supported by defective 2D–BN monolayer with a boron vacancy at 1000 fs during MD simulation at 1000 K. The temperature is controlled by using the NVT ensemble via a massive generalized Gaussian moments thermostat.

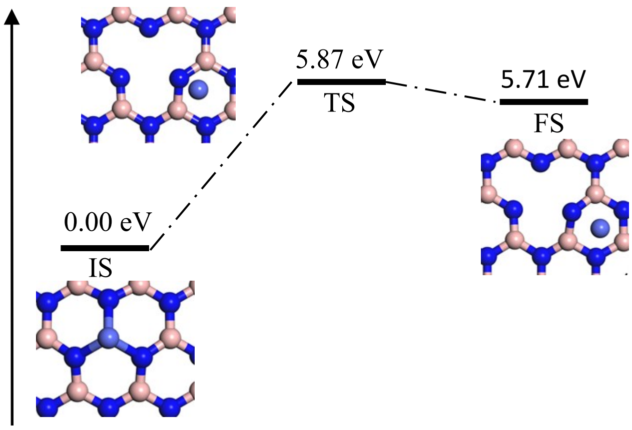


Fig. S2. The calculated initial state, transition state and product in the process of the transfer of a single Co atom from vacancy site to the neighboring hexagonal B_3N_3 ring.

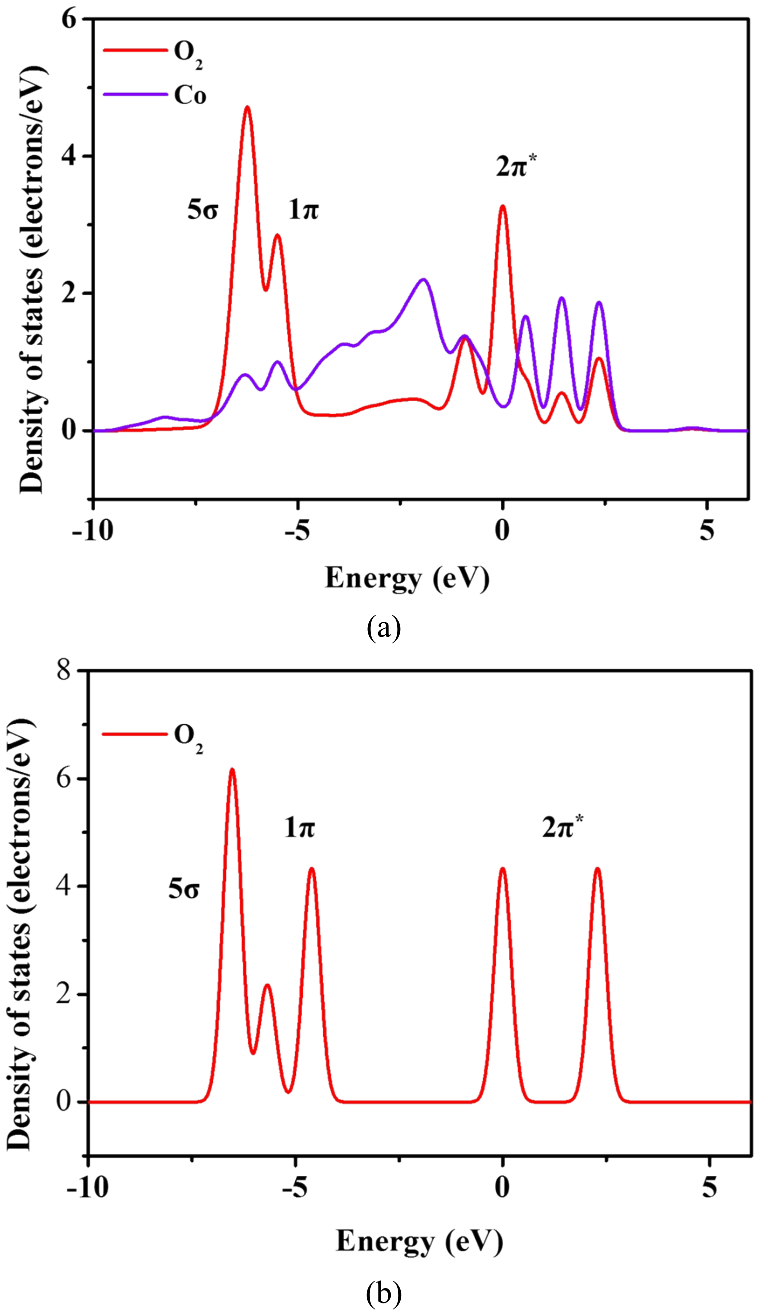
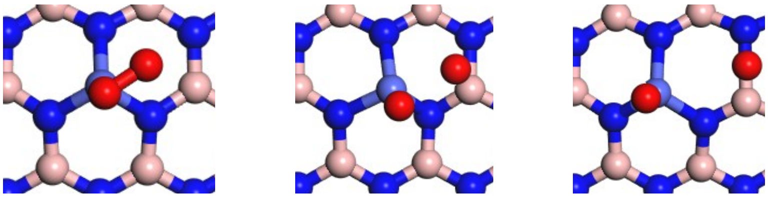
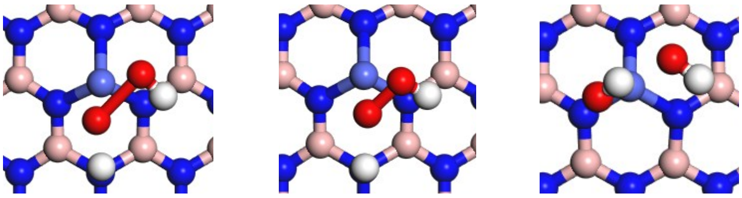


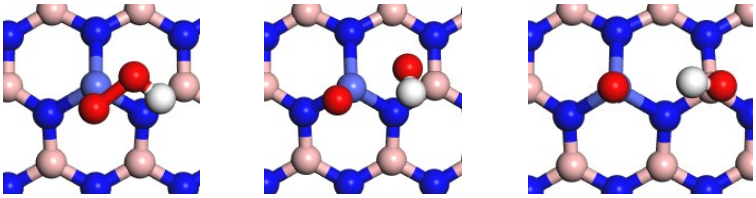
Fig. S3. The local density of states of O_2 adsorbed on the Co/BN surface (a) and gaseous O_2 (b).



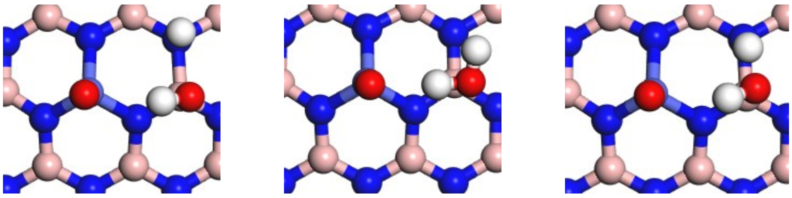
(1) a: $*O_2 \leftrightarrow 2*O$



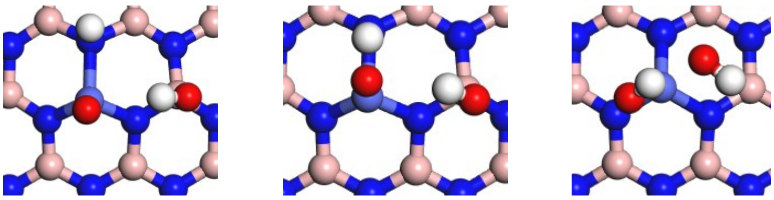
(2) c: $*OOH+H^+ +e^- \leftrightarrow 2*OH$



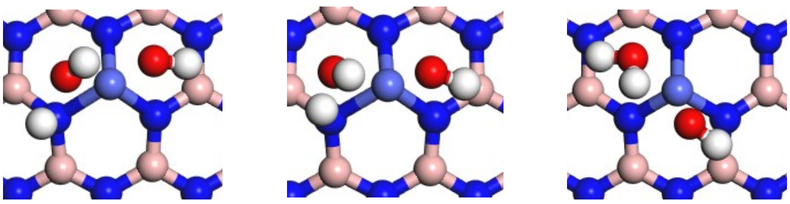
(3) g: $*OOH \leftrightarrow *O+*OH$



(4) h: $*O+*OH+H^+ +e^- \leftrightarrow *O+H_2O$



(5) i: $*O+*OH+H^+ +e^- \leftrightarrow 2*OH$



(6) j: $2*OH+H^+ +e^- \leftrightarrow *OH+H_2O$

Fig. S4. The optimized structures of initial state (left), transition state (middle) and final state (right) for the reaction step in Fig. 4.

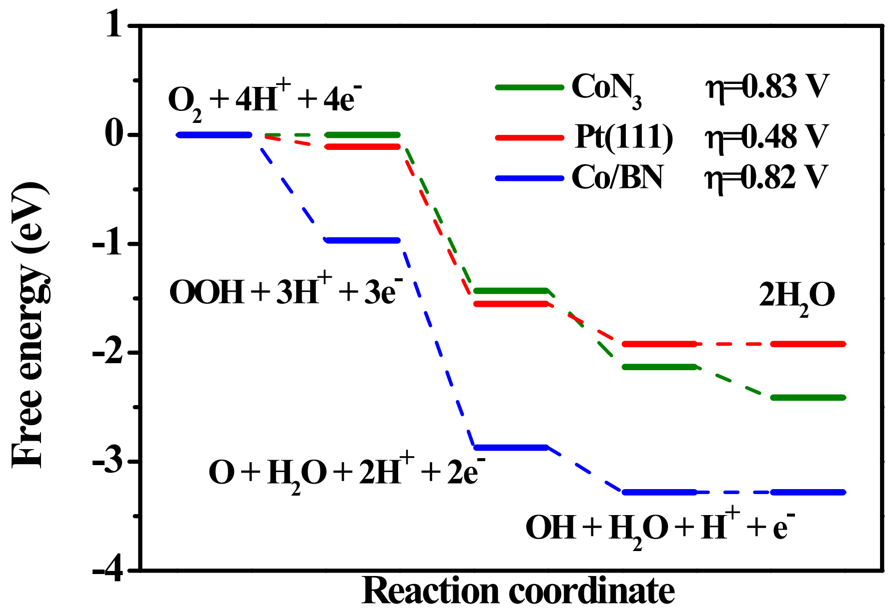


Fig. S5. Free energy diagrams for ORR on Pt (1 1 1) and CoN_3 embedded grapheme (CoN_3) and Co/BN catalyst.

The cutoff radius of 4.6Å was adopted by calculation the energy of the system varied with cutoff radius. As seen in following Fig. S6, the energy of the system maintain stable until the cutoff radius more than 4.6Å. On consideration of the calculation cost, 4.6Å was set as the cutoff radius in this work.

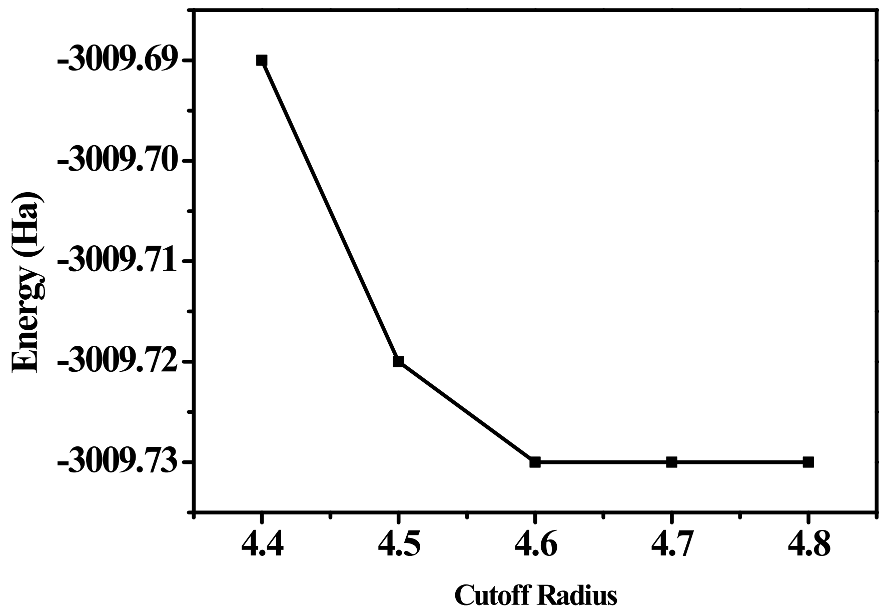


Fig.S6. The energy of the system varied with cutoff radius.

The schematic diagram of PEMFC shown in Fig. S7, H_2 is oxidized at anode and O_2 is reduced at cathode as expressed in following:

Anode: $H_2 \rightarrow 2H^+ + 2e^-$

H_2 is consumed at anode, producing H^+ and electrons for cathode.

Cathode: $1/2O_2 + 2H^+ + 2e^- \rightarrow H_2O$

The H^+ ions are conducted through the proton exchange membrane (PEM), and are combined with electrons and O_2 to form water at the cathode.

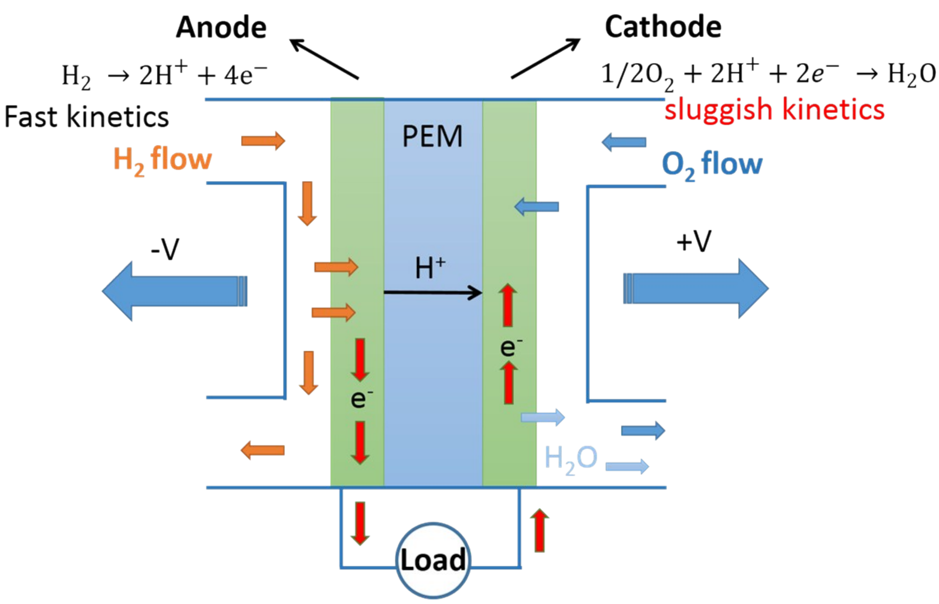


Fig. S7. Schematic diagram of PEMFC.