Electronic Supplementary Material (ESI) for Nanoscale.


# In-plane Graphene/Boron-Nitride Heterostructure as Efficient Metal-Free Electrocatalyst for the Oxygen Reduction Reaction

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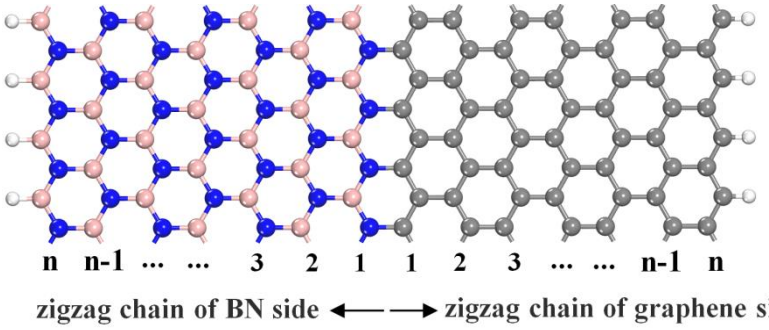
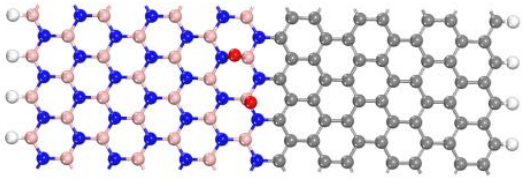
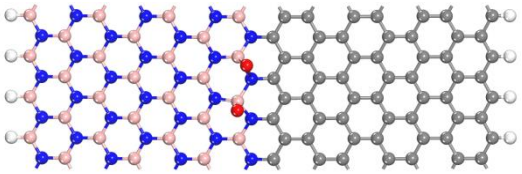


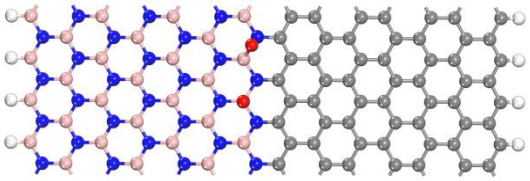

**Figure S1.** Geometry structure of zigzag type G/BN(n,n) nanoribbons.



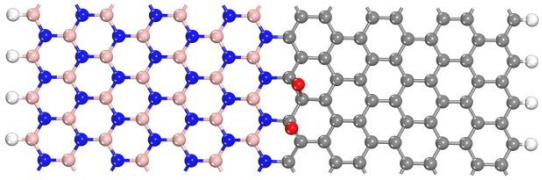
(a) O…O distance: 3.071 Å
Relative energy: 0.56 eV



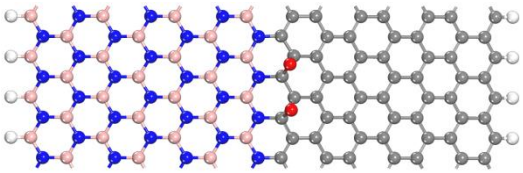
(b) O…O distance: 2.818 Å
Relative energy: 0.69 eV



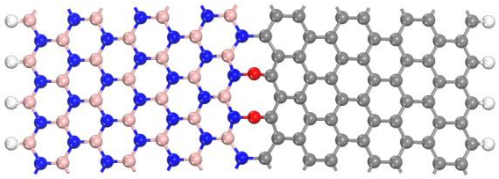
(c) O…O distance: 3.409 Å
Relative energy: 0.98 eV



(d) O…O distance: 2.685 Å
Relative energy: 0.04 eV

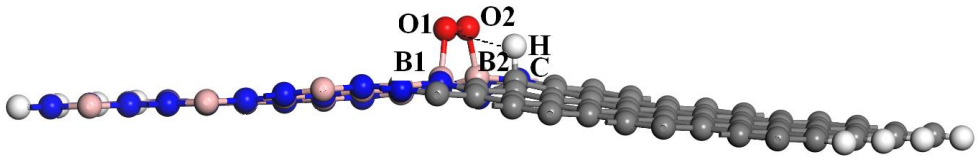


(e) O…O distance: 2.827 Å
Relative energy: 0.11 eV



(f) O…O distance: 2.655 Å
Relative energy: 2.48 eV

**Figure S2.** The optimized structures of the $O_2$ dissociation reaction.




O1…H distance: 2.340 Å

Relative energy: 0.54 eV

**Figure S3.** The structure (OO*…H*) of H binding to C atom at the interface of G/BN(7,7) nanoribbon.

**Table S1.** Mulliken charge distribution (e) of B atoms on the heterointerface of different sizes of G/BN nanoribbons and the changes in charge distribution before and after $O_2$ is adsorbed on the heterointerface of the G/BN nanoribbons, as well as the Mulliken charge distribution of O atoms for the chemisorption of $O_2$ on G/BN nanoribbons with different sizes.

| Index | Charge of B atom on the interface of G/BN | Charge of B atom on the interface of G/BN-$O_2$ | Change in charge of B atom on the interface of G/BN nanoribbon before and after $O_2$ adsorption | Charge of O atom on the G/BN-$O_2$ |
|---|---|---|---|---|
| G/BN (3,3) | 0.436 | 0.591 | 0.155 | -0.238 |
| G/BN (4,4) | 0.416 | 0.576 | 0.160 | -0.243 |
| G/BN (5,5) | 0.410 | 0.571 | 0.161 | -0.245 |
| G/BN (6,6) | 0.409 | 0.571 | 0.162 | -0.247 |
| G/BN (7,7) | 0.408 | 0.570 | 0.162 | -0.248 |
| G/BN (8,8) | 0.408 | 0.570 | 0.162 | -0.249 |
| G/BN (9,9) | 0.408 | 0.570 | 0.162 | -0.249 |
| G/BN (10,10) | 0.408 | 0.570 | 0.162 | -0.250 |

**Table S2.** Bond distance ($r$) in Å, binding energy ($E_{ad}$) in eV of $O_2$ adsorbed on G/BN nanoribbons with different sizes of graphene and BN as well as the charge transfer (CT) in electron from G/BN to $O_2$* of these configurations.

| index | r(O–O) | r(O–B) | r(B–B) | CT | $E_{ad}$ |
|---|---|---|---|---|---|
| G/BN (3,7) | 1.423 | 1.580 | 2.339 | -0.480 | -0.56 |
| G/BN (4,7) | 1.426 | 1.574 | 2.336 | -0.488 | -0.69 |
| G/BN (5,7) | 1.430 | 1.571 | 2.334 | -0.492 | -0.75 |
| G/BN (6,7) | 1.431 | 1.568 | 2.332 | -0.494 | -0.78 |
| G/BN (7,7) | 1.431 | 1.567 | 2.329 | -0.496 | -0.80 |
| | | | | | |
| G/BN (7,3) | 1.430 | 1.564 | 2.321 | -0.490 | -0.83 |
| G/BN (7,4) | 1.432 | 1.562 | 2.330 | -0.494 | -0.82 |
| G/BN (7,5) | 1.431 | 1.565 | 2.329 | -0.494 | -0.82 |
| G/BN (7,6) | 1.433 | 1.564 | 2.331 | -0.494 | -0.81 |
| G/BN (7,7) | 1.431 | 1.567 | 2.329 | -0.496 | -0.80 |