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

Supporting Information

Doped Boron Nitride Surfaces: Potential Metal Free Bifunctional Catalysts for Non-aqueous Li-O_2 Battery

*Chandra Chowdhury, Ayan Datta**

Department of Spectroscopy, Indian Association for the Cultivation of Science, Jadavpur- 700032,

West Bengal (India).

*** To whom correspondence should be addressed.**

Email: spad@iacs.res.in

Contents:

1. Partial density of states (PDOS) plots for doped h-BN surfaces.

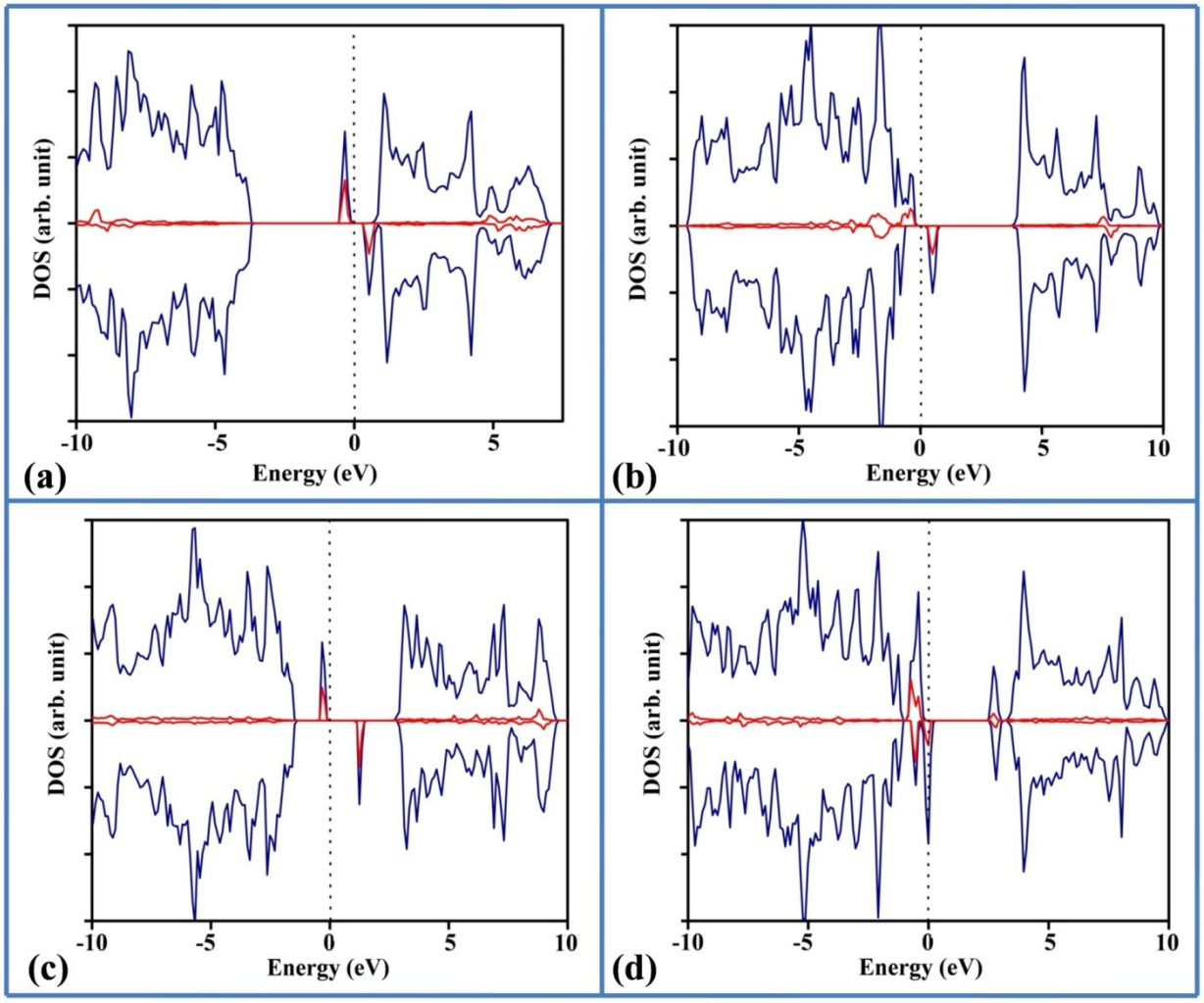

Figure S1: *Partial density of states of (a) C_B, (b) C_N, (c) Si_B and (d) Si_N-doped h-BN surfaces. Blue and red lines correspond to total density of states and dopant (C or Si) density of states, respectively.*

2. Band structures of P_B and P_N-doped h-BN using PBE functional.

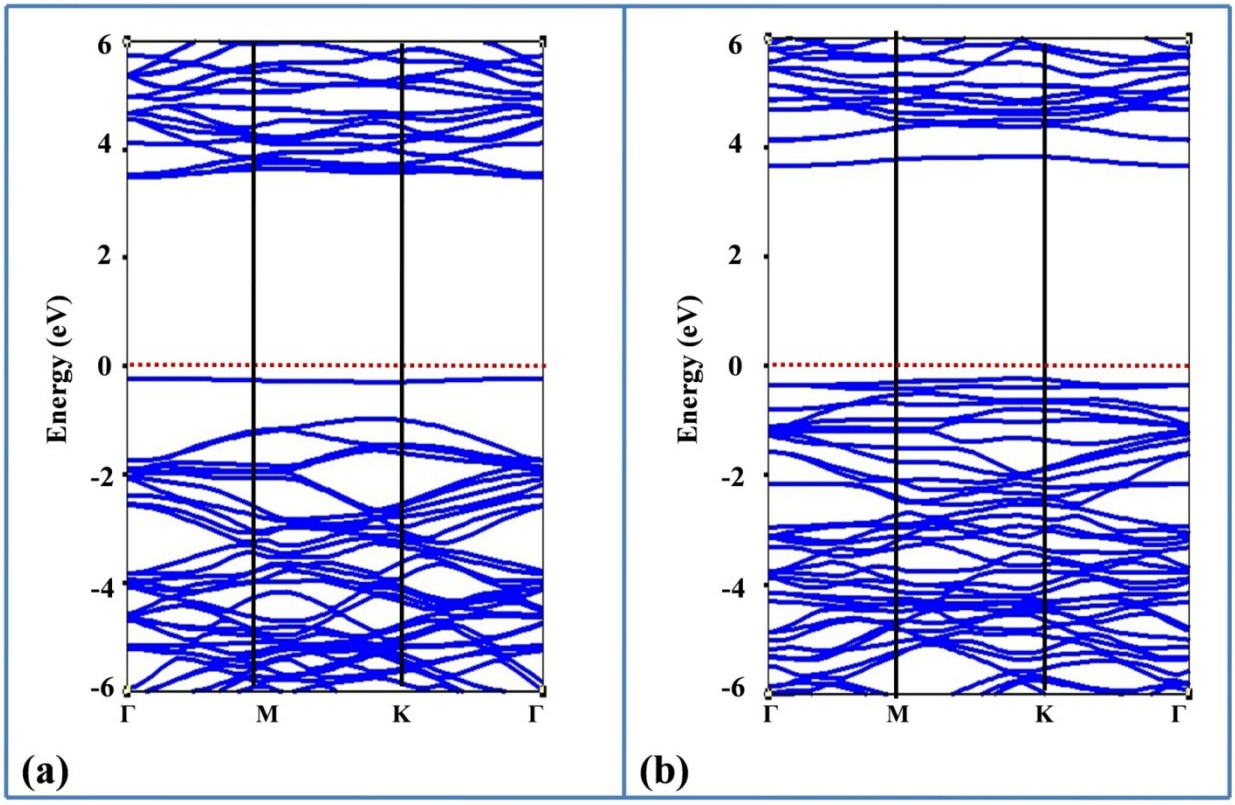

Figure S2: *Band structures of (a) P_B and (b) P_N-doped h-BN system calculated using PBE functional. Red dotted line corresponds to Fermi level.*

3. Adsorption energy profile diagram for C_B and C_N surfaces.

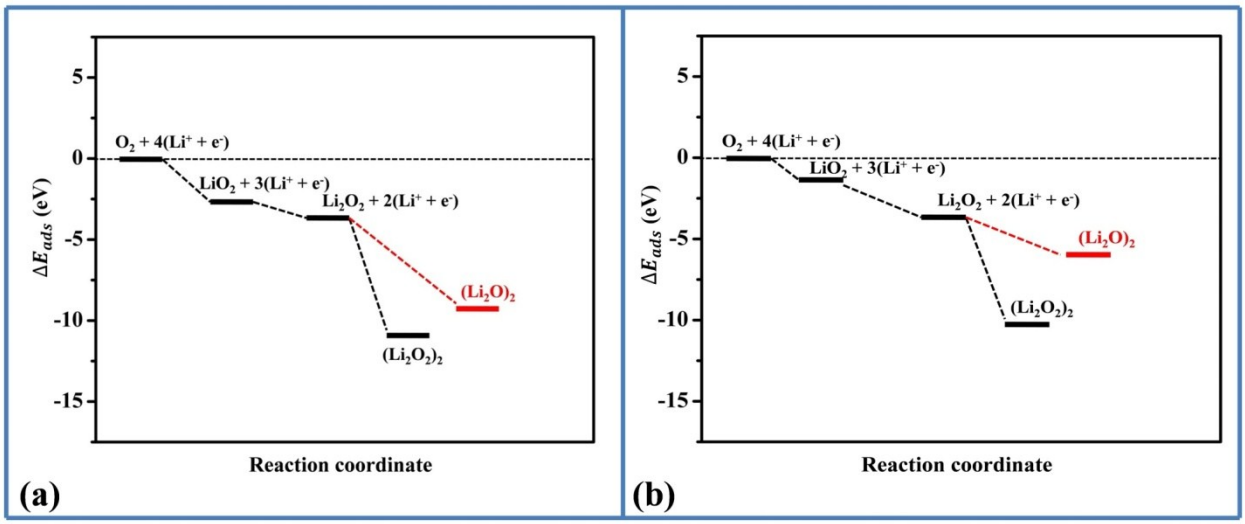

Figure S3: *Consecutive adsorption energy profile diagram for (a) C_B and (b) C_N surfaces with respect to reaction coordinate.*

4. Intermediate structures on different doped h-BN surfaces.

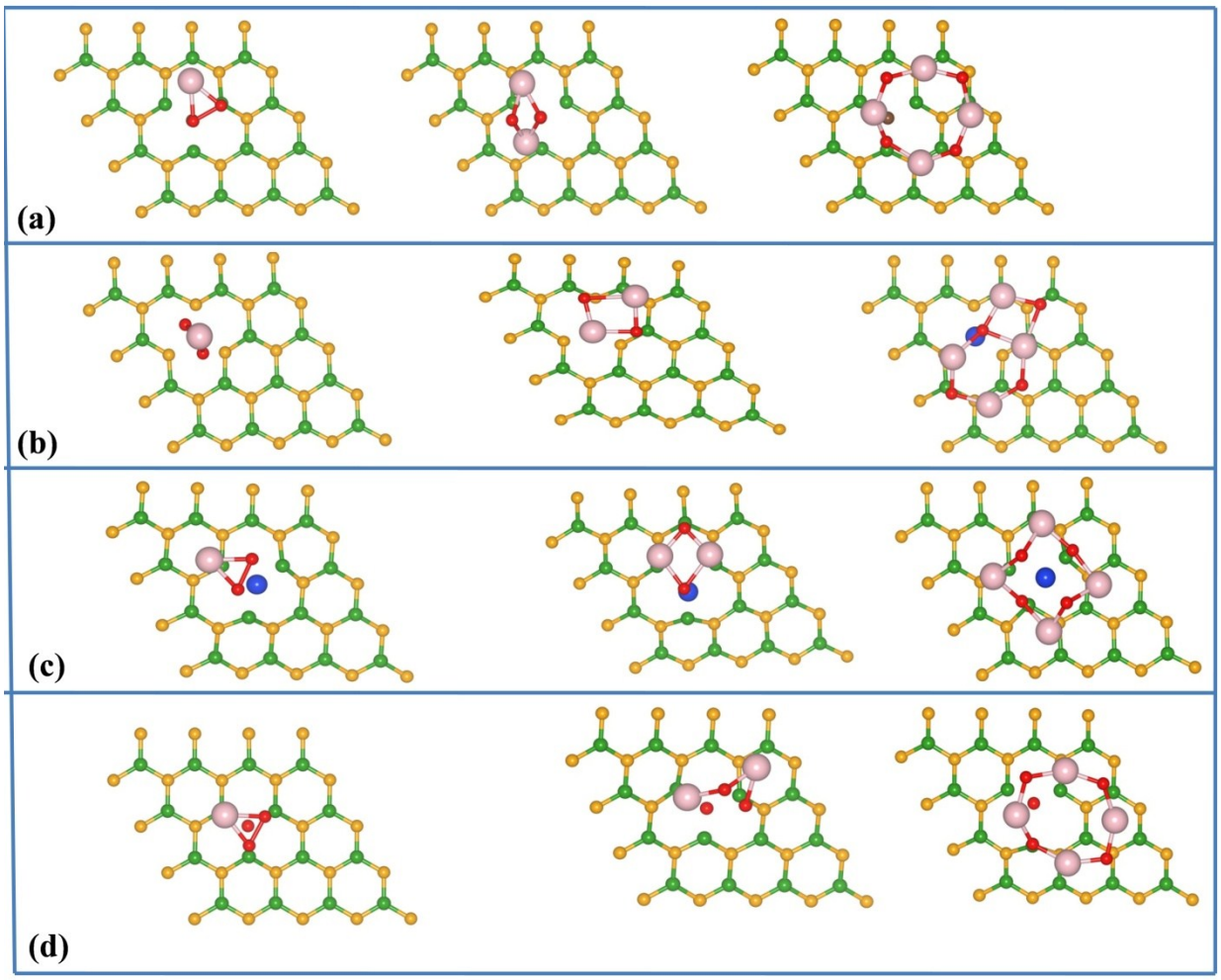

Figure S4: *Intermediate structures on (a) C_N, (b) Si_B, (c) Si_N and (d) O_N-doped h-BN surfaces.*

5. ***Table S1:*** *Charge distribution analysis of intermediate structures on C_B-doped h-BN surface.*

System	Adsorbate	Atom	Charge (e)
C_B	LiO_2	Li	+0.98
		O	-0.97
		O	-0.94
	Li_2O_2	Li	+0.98
		Li	+0.97
		O	-0.85
		O	-1.04
	Li_4O_2	Li	+0.98
		Li	+0.99
		Li	+0.96
		Li	+0.98
		O	-1.85
		O	-1.98
	Li_4O_4	Li	+0.98
		Li	+0.97
		Li	+0.99
		Li	+0.98
		O	-1.74
		O	-1.62
		O	-0.99
		O	-0.99

6. Initial and final structures for NEB calculation on C_B, Si_B and O_N surfaces.

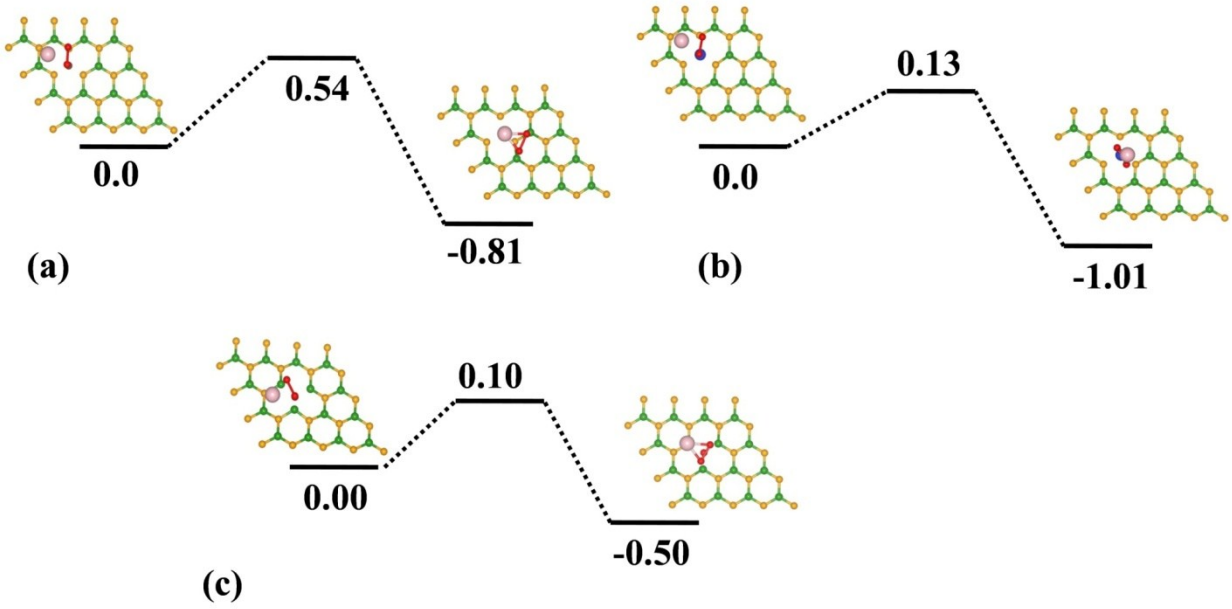

Figure S5: *Initial and final structures for (a) C_B, (b) Si_B and (c) O_N in NEB calculation.*

7. Free energy diagrams on different surfaces.

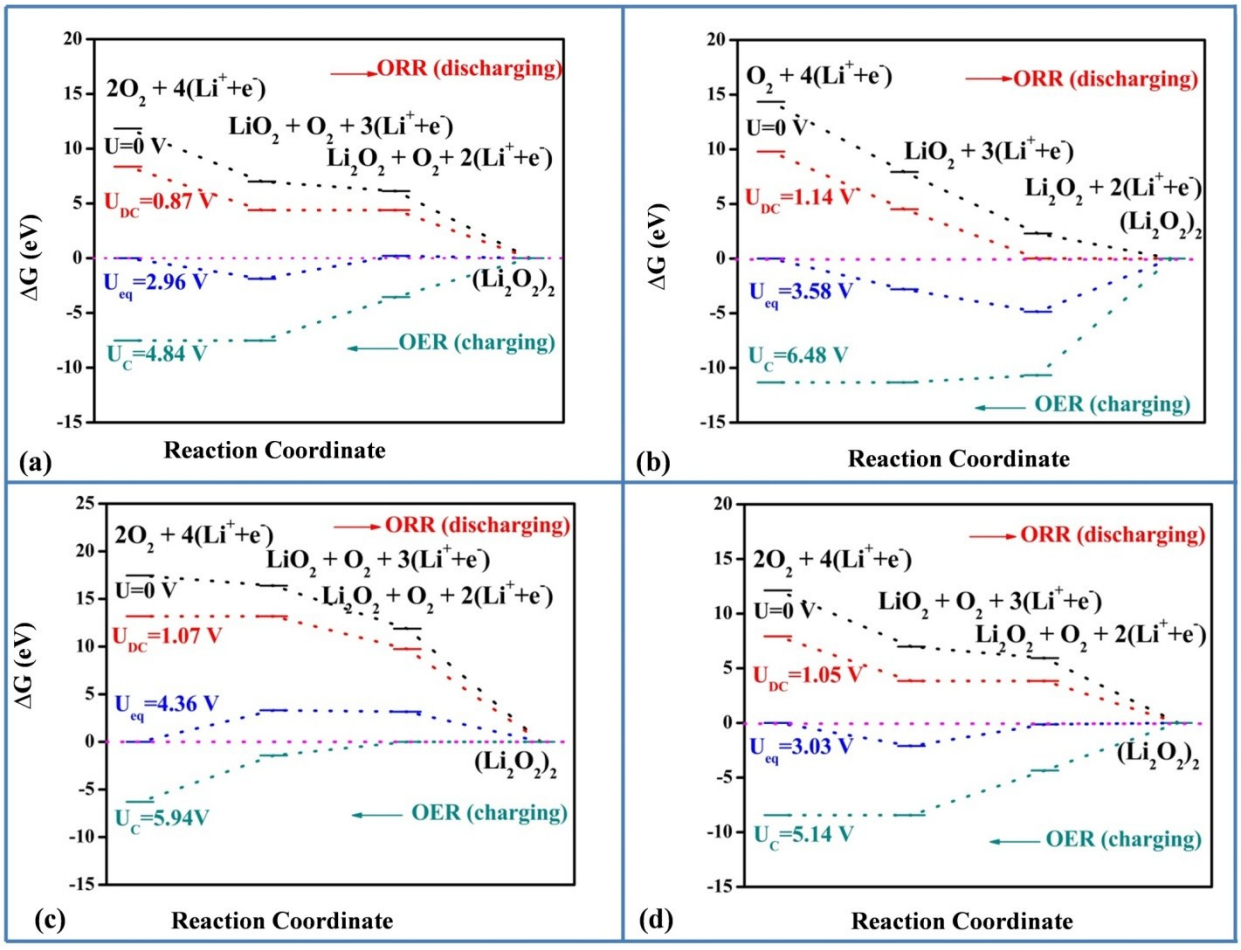

Fig S6: *Free energy diagram of (a) C_B, (b) Si_B, (c) Si_N and (d) O_N surfaces.*

8. Band structures of Li_4O_4 adsorbed C_N surface.

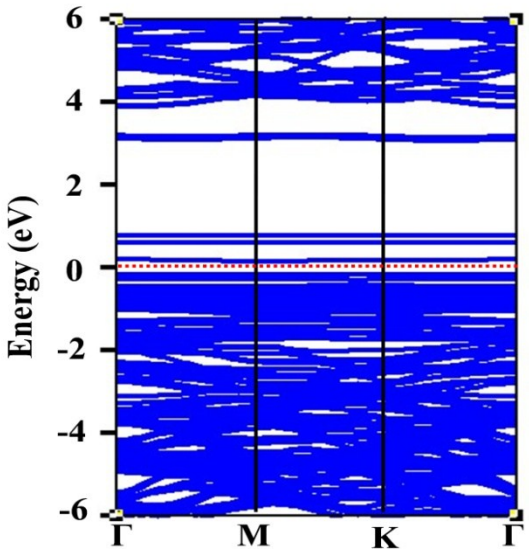

Figure S7: *Band structures of C_N surface adsorbed with Li_4O_4.*