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

ELECTRONIC SUPPLEMENTARY INFORMATION

Theoretical insights on structural, electronic and thermoelectric properties of inorganic biphenylene monolayer

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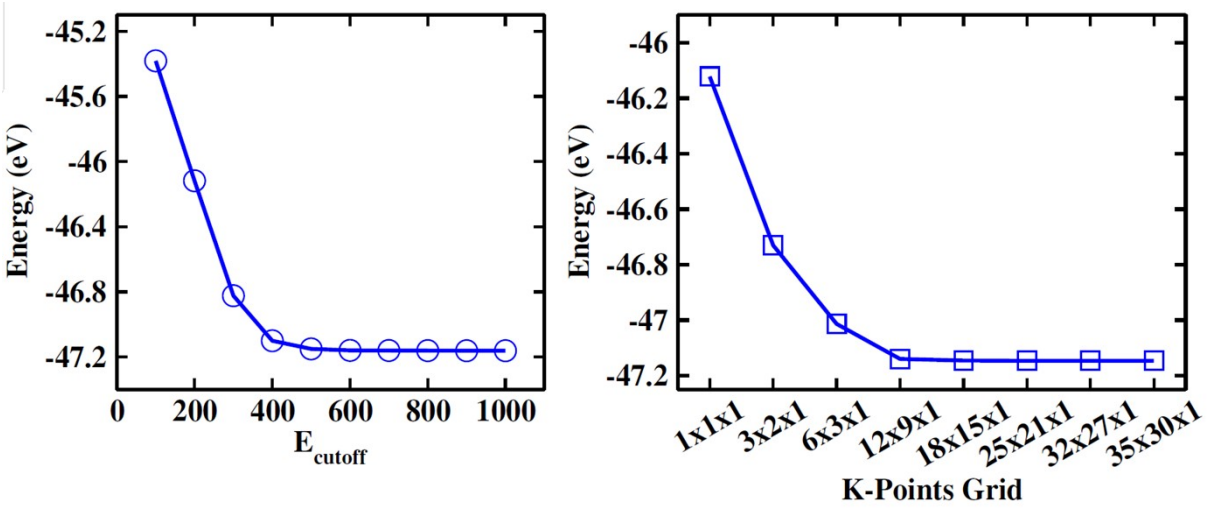


Fig S1: The energy convergence test for plane wave energy cutoff (left) and K-points grid (right)

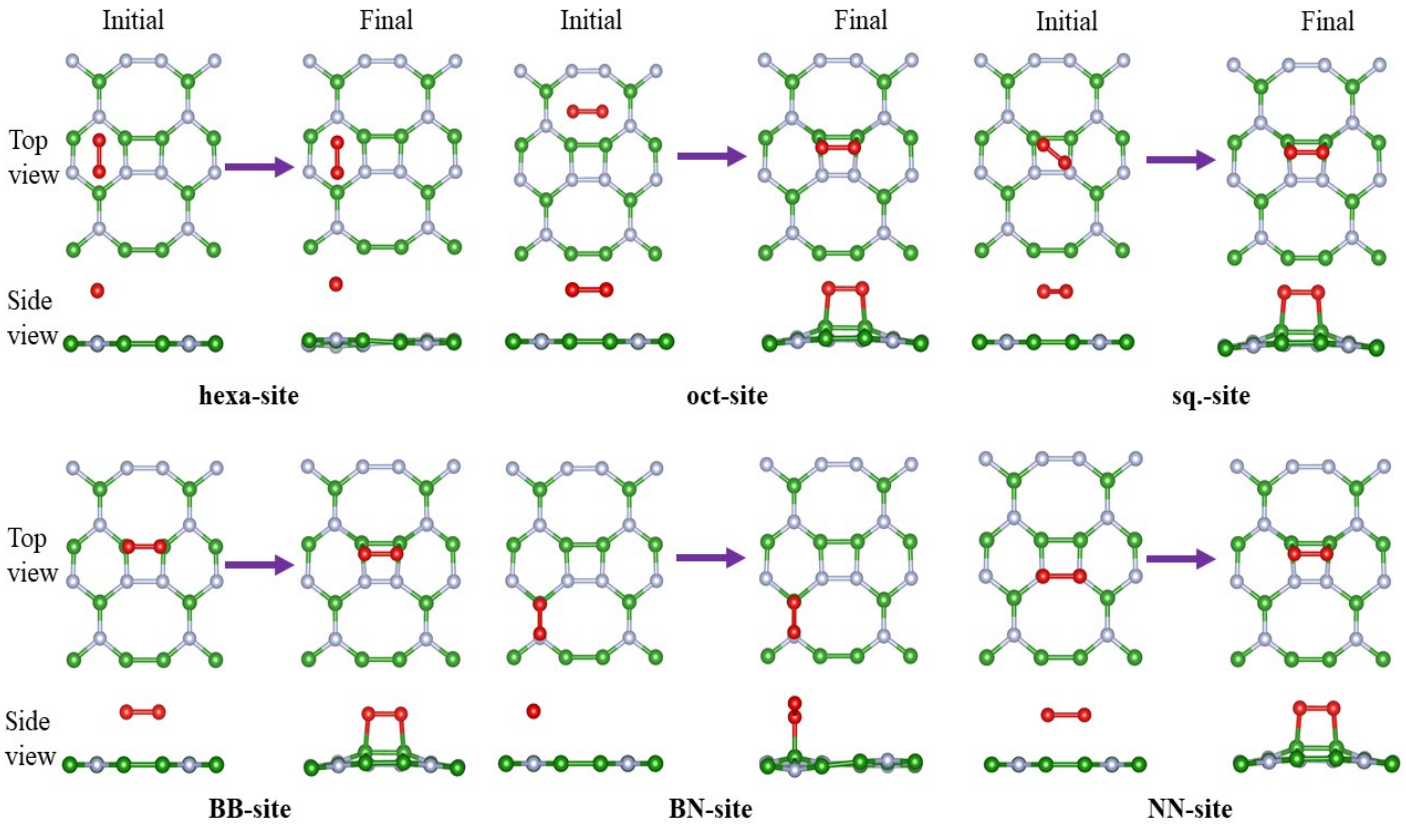
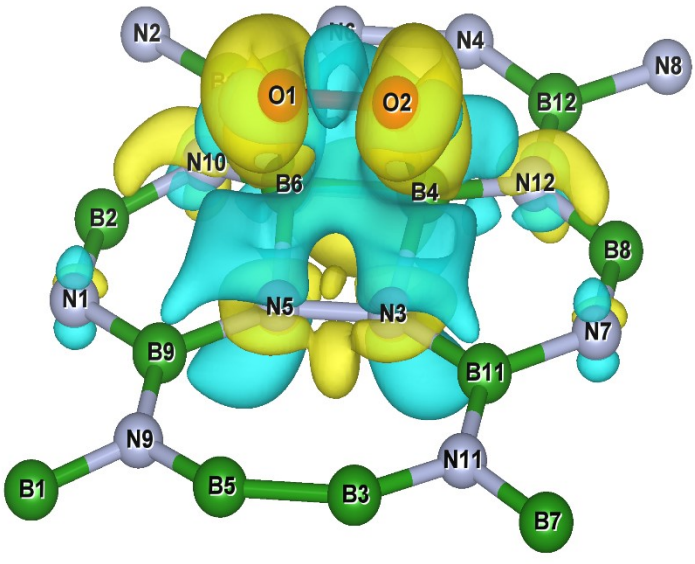


Fig S2: The initial (before relaxation) and final (after relaxation) structures of oxygen molecule (O_2) adsorbed at all possible sites of the I-BPN monolayer.

Table S1 reports the net Bader charge on each atom for both the pristine and oxygen-adsorbed I-BPN monolayer. The figure on the right side of Table S1 displays the labels for all atoms.

Atoms	Net charge in pristine I-BPN and O_2	Net charge in O_2 adsorbed I-BPN at BB-site	Net Charge transfer
B1	1.92	1.92	0
B2	1.9	1.91	0.01
B3	1.92	1.92	0
B4	1.85	1.98	0.13
B5	2.02	2.02	0
B6	1.95	2.07	0.12
B7	2.02	2.02	0
B8	2.01	2.01	0
B9	3	3	0



B10	3	3	0
B11	3	3	0
B12	3	3	0
N1	-1.96	-1.9	0.06
N2	-1.96	-1.94	0.02
N3	-1.84	-1.52	0.32
N4	-1.96	-1.93	0.03
N5	-1.69	-1.36	0.33
N6	-1.85	-1.82	0.03
N7	-1.84	-1.79	0.05
N8	-1.85	-1.83	0.02
N9	-3.13	-3.11	0.02
N10	-3.14	-3.12	0.02
N11	-3.12	-3.11	0.01
N12	-3.14	-3.12	0.02
O1	0	-0.66	-0.66
O2	0	-0.65	-0.65

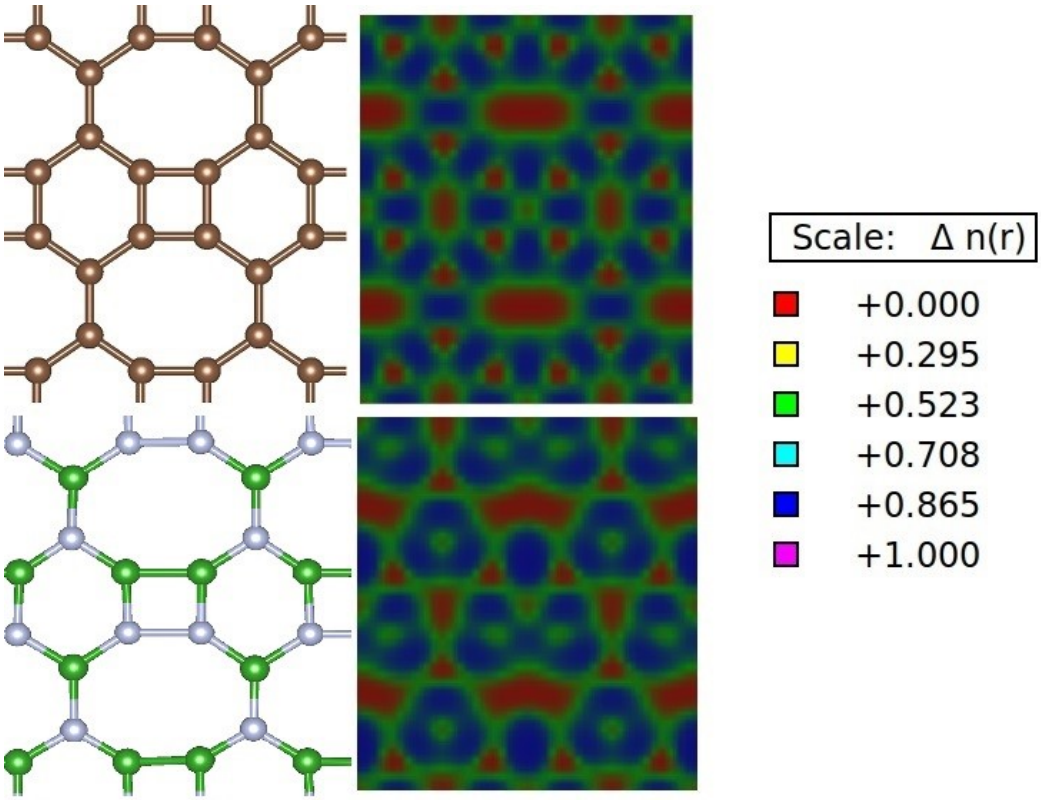


Fig S3: The BPN and I-BPN structures and their corresponding electron localized function plots with an iso-surface of 0.02 eV/Å

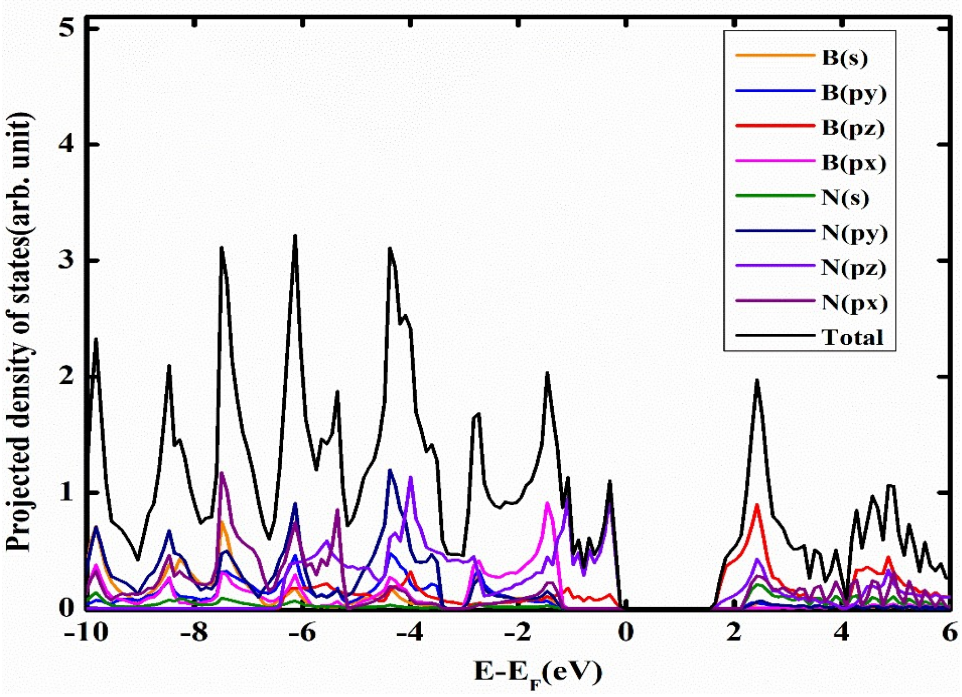


Fig S4: projected density of states of I-BPN

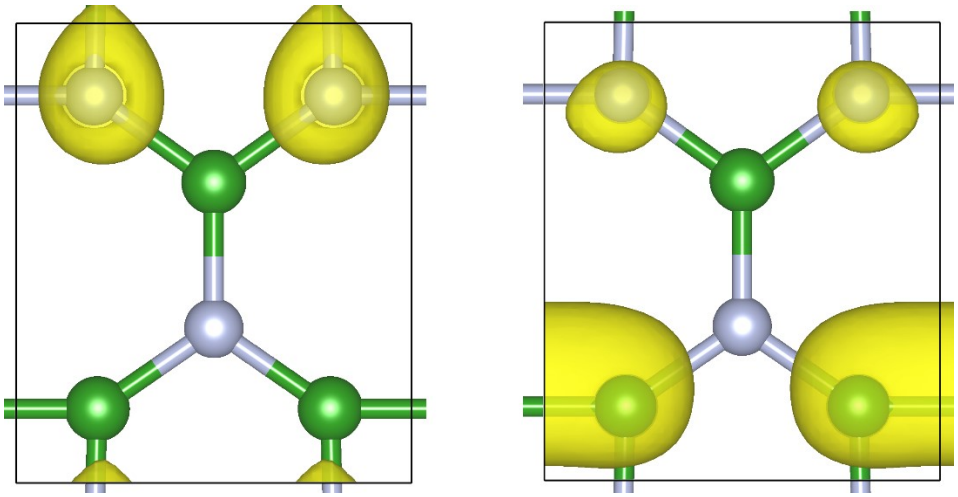


Fig S5: The Valence band maximum (left) and conduction bands minimum (right) of the electronic band structure of I-BPN per unit cell.