Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information:

Adsorption of singlet and triplet oxygen on B-doped graphene: Adsorption and electronic characteristics

A. Sahithi and K. Sumithra*
Department of Chemistry, Birla Institute of Technology and Science, Pilani, Hyderabad Campus, 500078 Hyderabad, India.

*Author to whom correspondence should be addressed.
Electronic mail: sumithra@hyderabad.bits-pilani.ac.in

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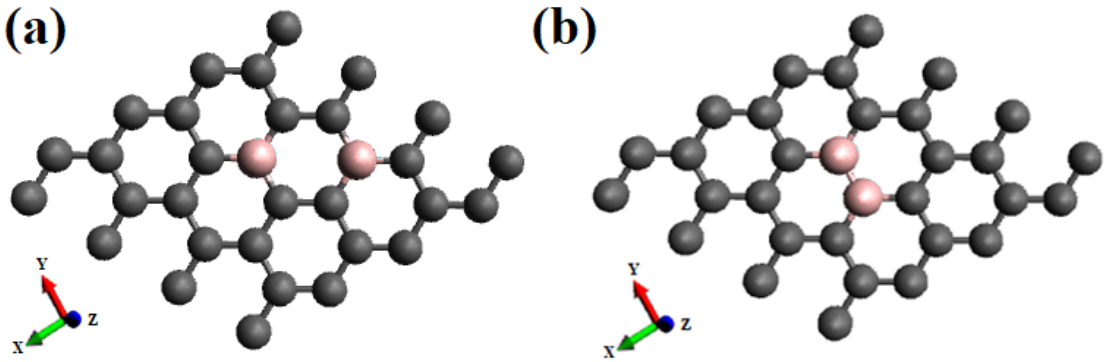

Fig. S1 The 4 × 4 boron doped graphene supercell configurations with different concentrations of 6.25% boron, (a) and (b) denoted, as B2G-1 and B2G-3 respectively.

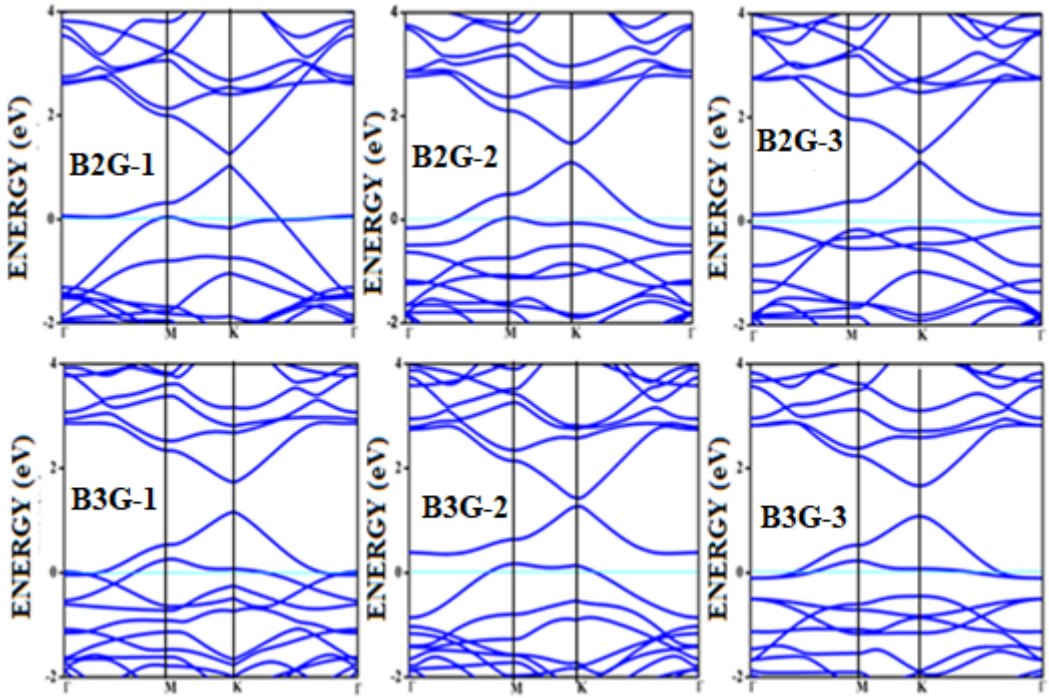

Fig. S2 The band structures of borons doped graphene different patterns with different concentrations of doping shown in Fig. 1, in the manuscript and Fig. S1.

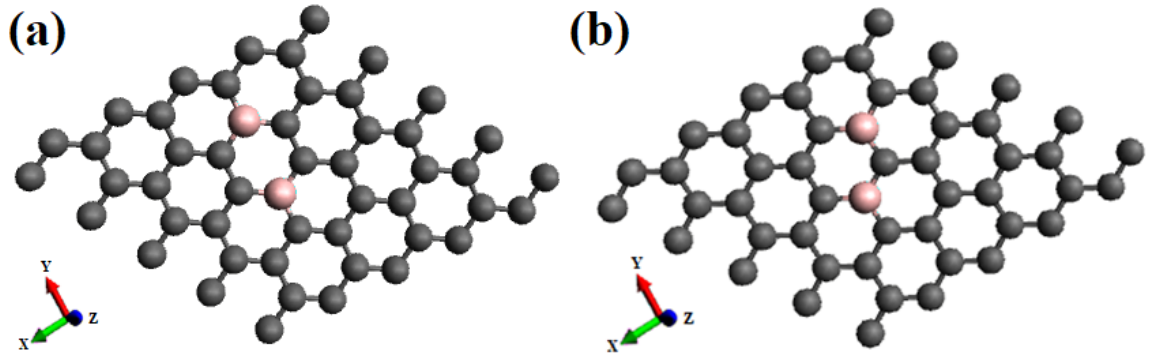

Fig. S3 The optimized 5 × 5 boron doped graphene supercell with concentration of 4% with different configurations from (a) and (b) denoted as B2G-1/5 × 5 and B2G-2/5 × 5.

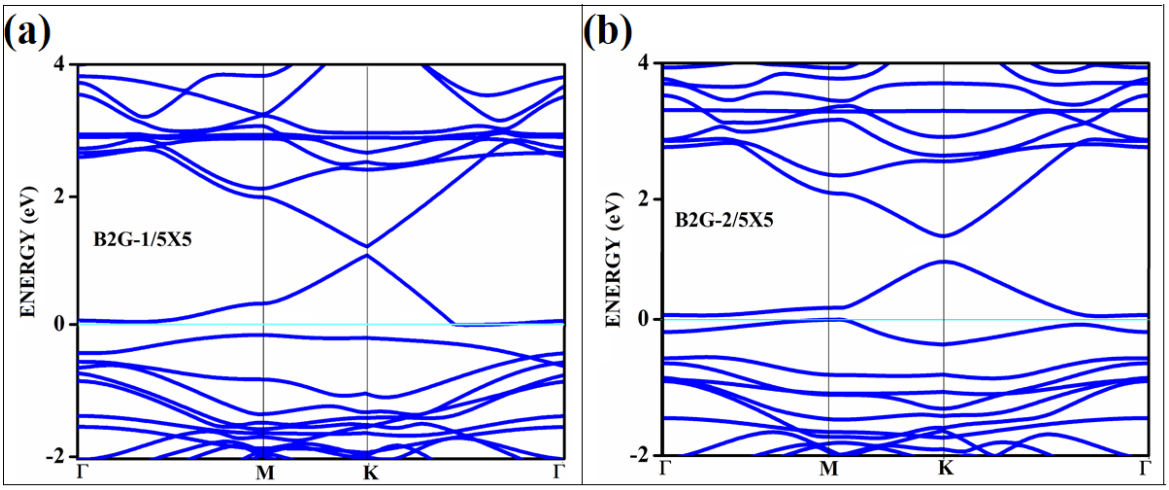

Fig. S4 The band structures borons doped graphene supercell of configurations with doping percent of 4% as shown in Fig. S3.

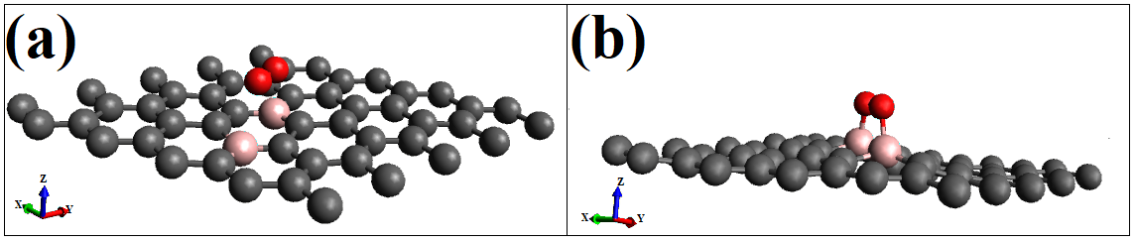

Fig. S5 Shows the optimized geometries of respective singlet O_2 adsorption on modified graphene surfaces (a) O_2(s)/B2G-1/5 × 5 (b) O_2(s)/B3G-2/5 × 5.

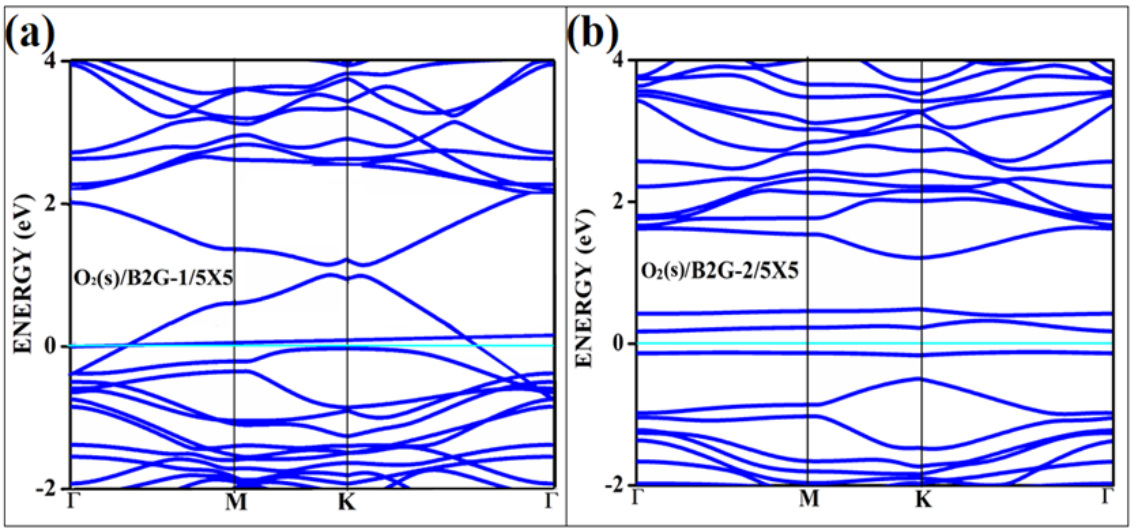

Fig. S6 Shows the band structure of oxygen in singlet state adsorbed on surfaces (a) O_2(s)/B2G-1/5 × 5 (b) O_2(s)/B2G-2/5 × 5 ((s); singlet state of oxygen).

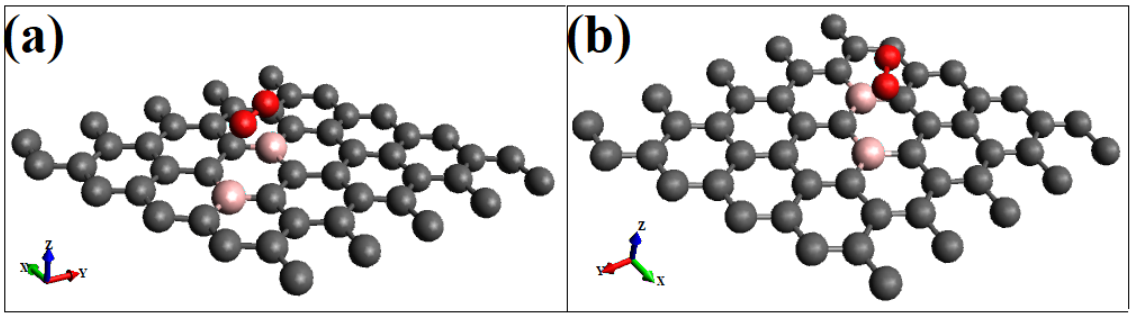

Fig. S7 The optimized geometries of respective triplet O_2 adsorption on modified graphene surfaces (a) O_2(t)/B2G-1/5 × 5 (b) O_2(t)/B3G-2/5 × 5.

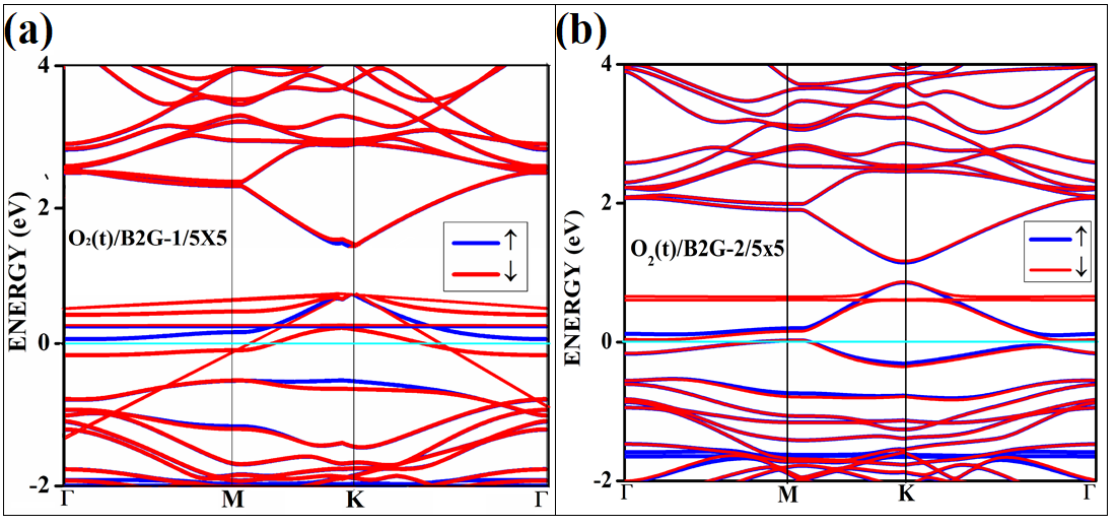

Fig. S8 The band structure of oxygen in triplet state adsorbed on surfaces (a) O2(t)/B2G-1/5 × 5 (b) O2(t)/B2G-2/5 × 5 ((t); triplet state of oxygen).

Table S1. The adsorption energy, distance of adsorbate from the adsorbent, band gaps and the Bader charge transfers of oxygen in singlet state adsorption on 5 × 5 supercell, 4% boron doped graphene were given respectively. Shown in parenthesis are the values obtained for 6.25% boron concentration on 4 × 4 supercell.

System $^1\Delta_g$ on 5x5	Adsorption energy (eV)	Distance (Å)	Charge transfer (e)
B2G-1 (B-C-C-B)	-0.752 (-0.664)	2.0 (1.9)	0.06(0.06)
B2G-2 (B-C-B)	-1.152 (-1.222)	1.53 (1.53)	0.34 (0.32)

Table S2. The adsorption energy, distance of adsorbate from the adsorbent, band gaps and the Bader charge transfers of oxygen in triplet state adsorption on 5 × 5 supercell boron doped graphene were given respectively.

System $^3\Sigma_g$ on 5x5	Adsorption energy (eV)	Distance (Å)	Band gap (eV)	Charge transfer (e)
B2G-1 (B-C-C-B)	-0.154 (-0.144)	2.80 (2.86)	-	0.02 (0.02)
B2G-2 (B-C-B)	-0.146(-0.138)	2.85(2.9)	0.39(0.41)	0.04(0.04)

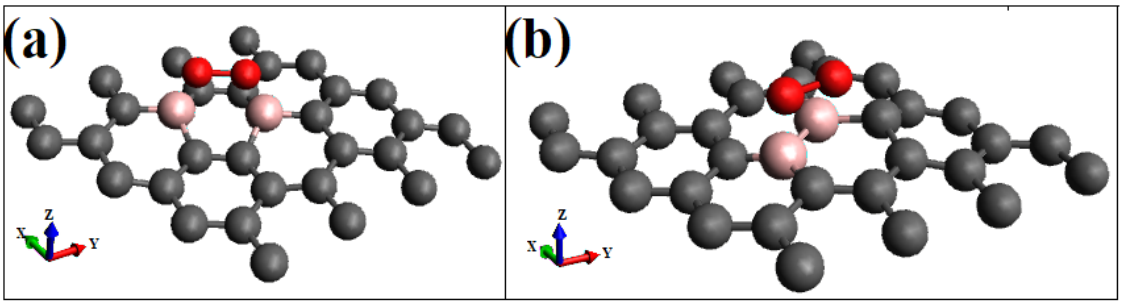

Fig. S9 Shows the optimized geometries of respective singlet O_2 adsorption on modified graphene surfaces (a) O_2(s)/B2G-1 (b) O_2(s)/B3G-3.

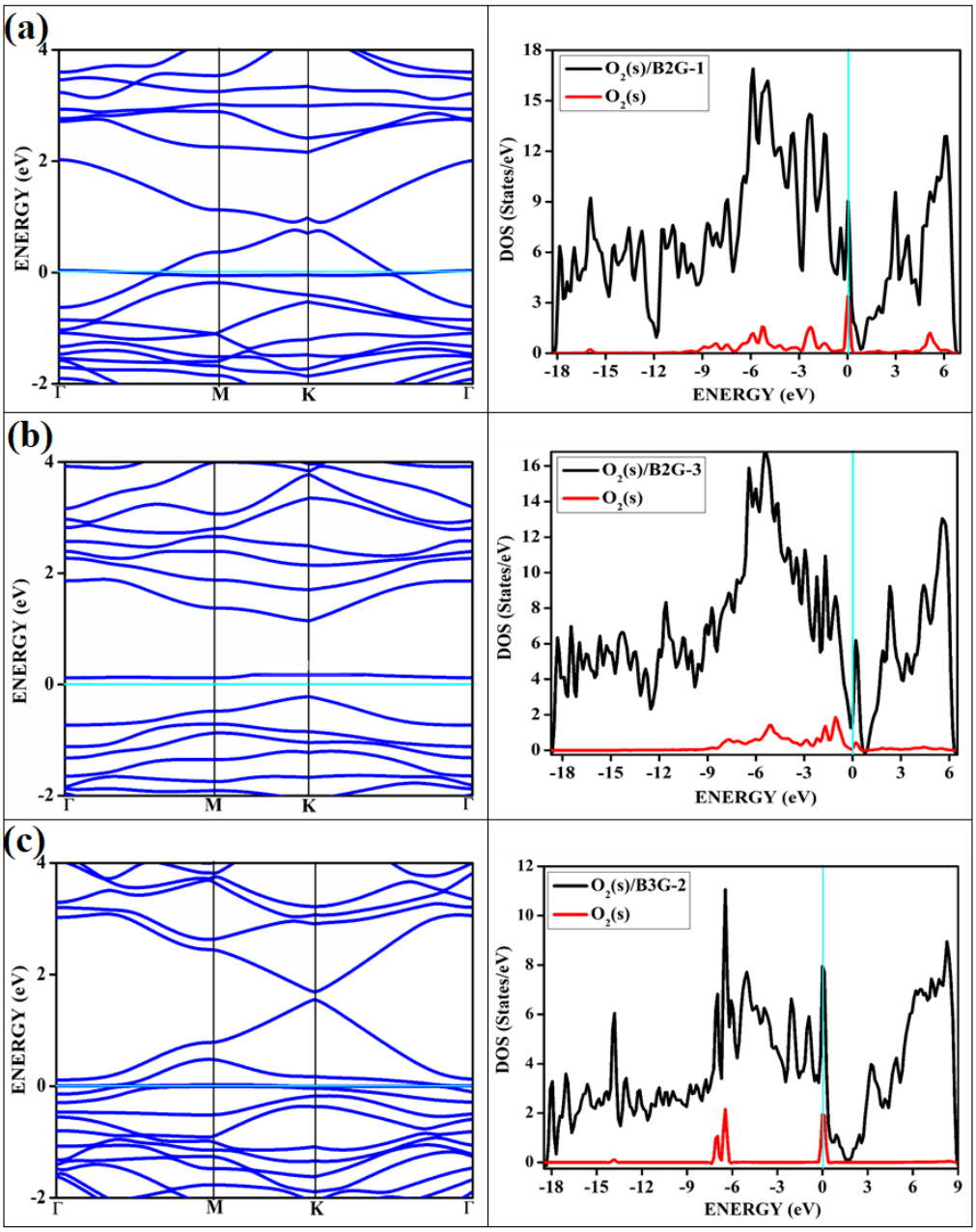

Fig. S10 Shows the band structure and corresponding DOS of oxygen in singlet state adsorbed on surfaces (a) O_2(s)/B2G-1 (b) O_2(s)/B2G-3 (c) O_2(s)/B3G-2 ((s); singlet state of oxygen). The magenta, red and blue represent the PDOS of carbon, oxygen and boron respectively.

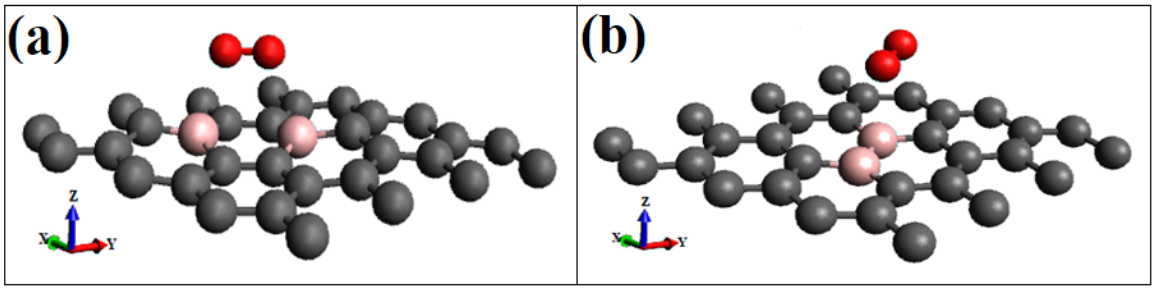

Fig. S11 Shows the optimized geometries of respective triplet O_2 adsorption on modified graphene surfaces (a) O_2(t)/B2G-1 (b) O_2(t)/B3G-3.

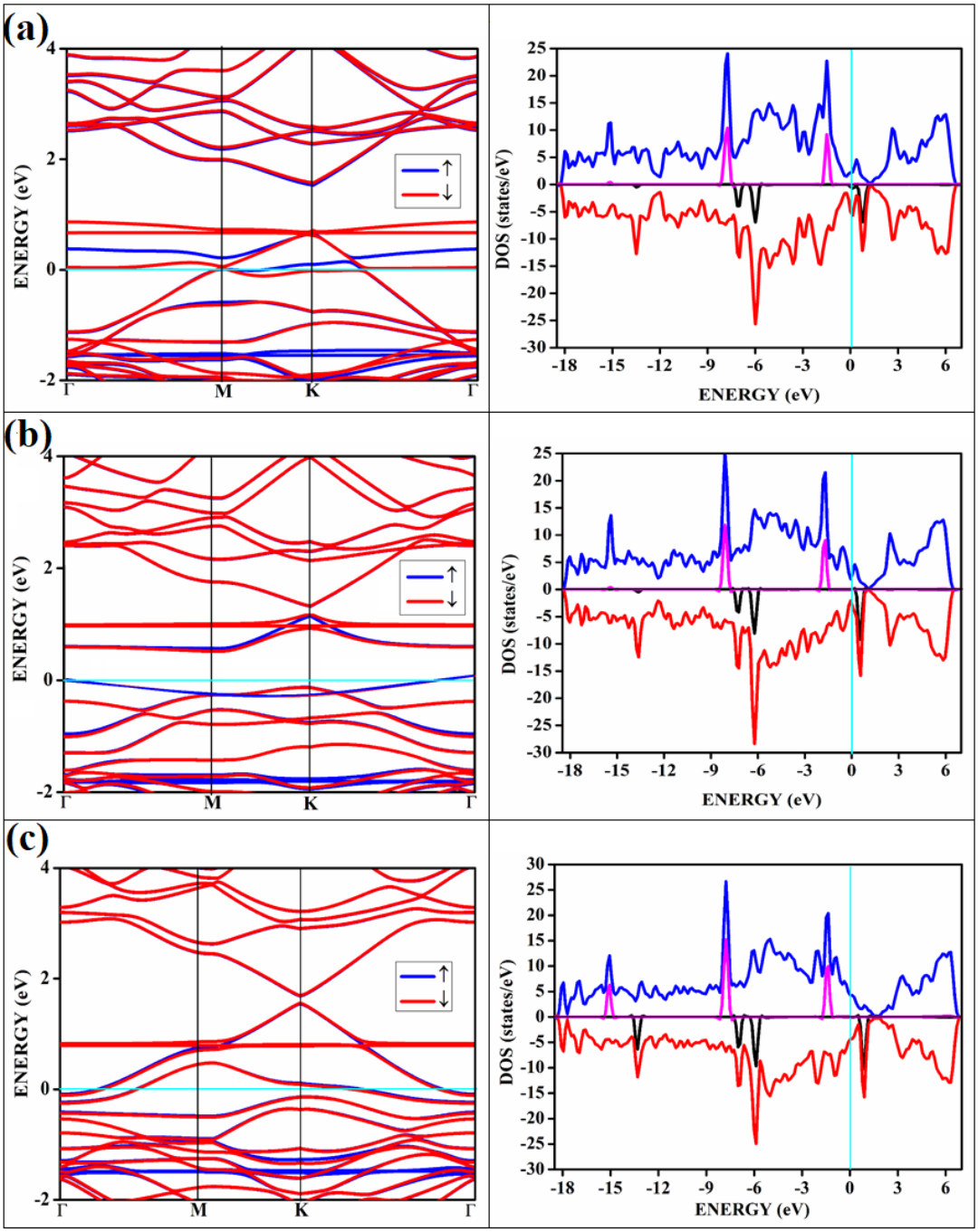

Fig. S12 Shows the band structure and corresponding DOS of oxygen in triplet state adsorbed on surfaces (a) O_2(t)/B2G-1 (b) O_2(t)/B2G-3 (c) O_2(t)/B3G-2 ((t); triplet state of oxygen). The magenta and black correspond to the PDOS of oxygen.