

Supporting information for:  
**Boron-Doped Graphene Topological Defects:  
Unveiling High Sensitivity to NO Gas  
Molecules for Gas Sensing Applications**

B Keshav Rao<sup>a</sup>, Tadeu Luiz Gomes Cabral<sup>b</sup>, Debora Carvalho de Melo Rodrigues<sup>c</sup>, Fábio A. L. de Souza<sup>d</sup>, Wanderlã L. Scopel<sup>e</sup>, Rodrigo G. Amorim<sup>b</sup>, Ravindra Pandey<sup>f</sup>

<sup>a</sup>*Department of Applied Physics, Shri Shankaracharya Technical Campus, Junwani, Bhalai, 490020, Chhattisgarh, India*

<sup>b</sup>*Universidade Federal Fluminense, R. Des. Ellis Hermydio Figueira, 783 - Aterrado, Volta Redonda, 27213-145, Brazil*

<sup>c</sup>*Departamento de Física, Universidade Federal Instituto de Física, Universidade Federal Fluminense, Av. Litorânea, sn, Niterói, 24210-340, RJ, Brazil*

<sup>d</sup>*Departamento de Física, Federal Institute of Education, Science and Technology of Espírito Santo, Ibatiba, 29395-000, ES, Brazil*

<sup>e</sup>*Departamento de Física, Universidade Federal do Espírito Santo, Vitória, 29075-910, ES, Brazil*

<sup>f</sup>*Department of Physics, Michigan Technological University, Houghton, 49931, Michigan, USA*

---

*Keywords:* B-doping line defect in graphene, Density Functional Theory, Green's Function, Simulated Scanning Tunneling Microscopy, Electron Transport, Gas Sensing.

---

Table S1: Dopant substitutional energies of B impurity in graphene with line defect unit cell. B-doped adsorption sites according to Figure 1. The most stable site is set as zero.

B-doped Sites	1	2	3	5
$\Delta E$ (eV)	0.10	0.00	0.71	0.14

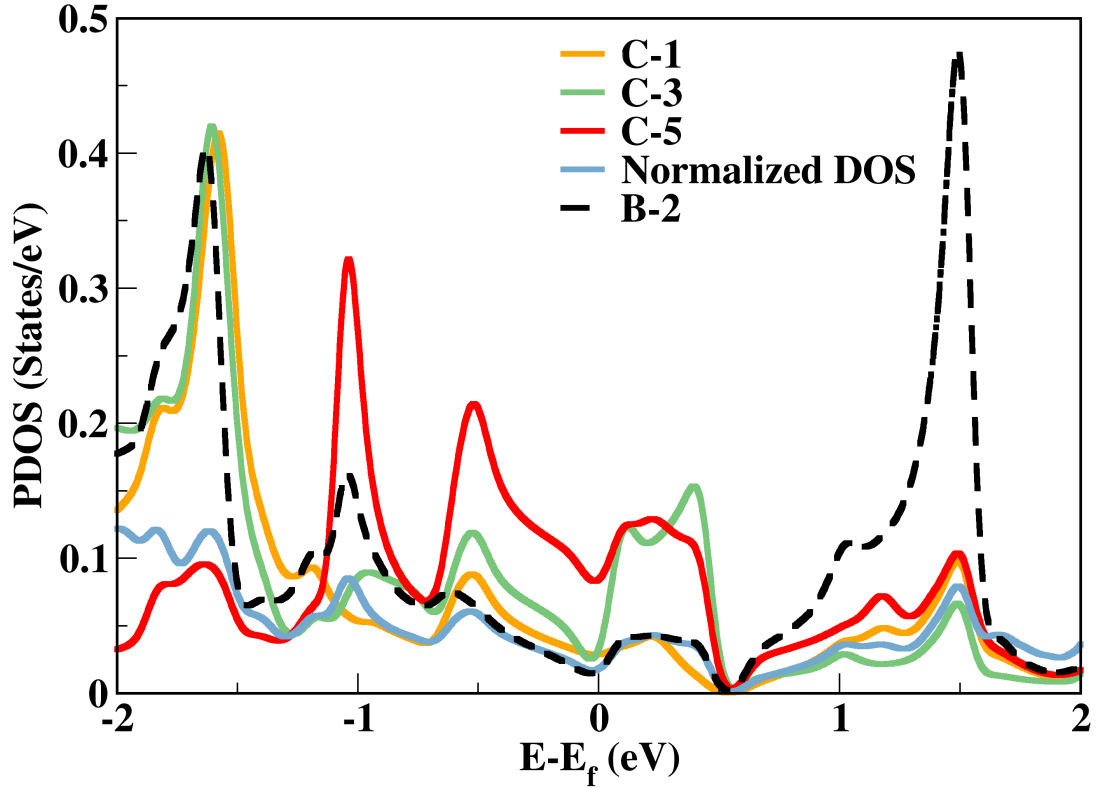


Figure S1: The calculated projected density of states for B-doped defective graphene. B atom occupies the most stable site (2), where  $C_1$ ,  $C_3$ , and  $C_5$  atoms are the first neighbors of it. The total dos normalized by the total number of atoms is also shown.

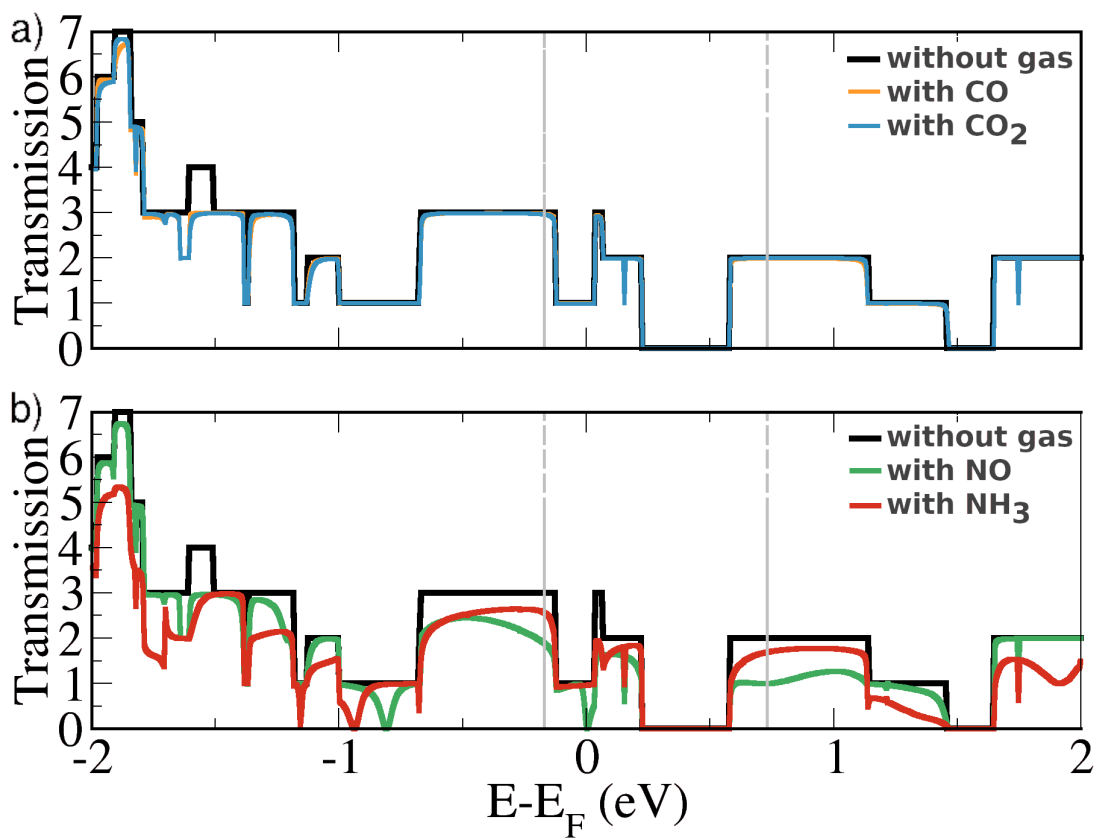


Figure S2: Zero bias transmission as a function of the energy for the B-doped line defect in graphene device with and without gas molecule a) CO and CO<sub>2</sub> gas; b) NO and NH<sub>3</sub> gas.