Adsorption of helium on graphene:
A density functional theory investigation

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INTRODUCTION
Radioactive environments generate microstructural changes and mechanical properties deterioration in the materials that constitute nuclear reactors. In addition, the presence of trapped helium degrades the behavior of the materials and promotes the embrittlement of these [1]. Therefore, finding a material capable of minimizing the radiation damage is very desirable.

Graphene has become one of the most important materials in the field of nanoscience due to its many applications. The reduced thickness, the high mechanical strength and the impermeability for He of this material [2], in addition to its mechanical, thermal and chemical stability, make graphene a potential candidate for the shielding of nuclear reactors against radiation prolonging its shelf life [3].

The present work focuses on the adsorption of helium on graphene. To study the saturation and diffusion of helium on graphene, we have employed density functional theory (DFT).

METHODOLOGY
With the aim of studying the saturation of He as close as possible to reality, the next procedure has been followed:

1. Generate a 4x4x1 graphene supercell with ASE.
2. Add helium atoms successively above hexagons center (C), midpoint of hexagons sides, or bridge (B), and hexagons vertices (V) belonging to the graphene sheet with the purpose of finding out the arrangements with the minimum energy.
3. Perform a self-consistent calculation for electrons and a ionic relaxation not allowing the cell to vary using the Quantum Espresso code.
4. Use the ionic positions obtained at the end of each calculation in the immediately next calculation in which we have added another helium atom.

RESULTS

Figure 3 Arrangement of adsorbed He atoms on graphene in an intermediate step before achieving the saturation and their corresponding adsorption energies listed in the accompanying table. The most favorable diffusion paths of He on graphene have been studied too.

<table>
<thead>
<tr>
<th>He Atom</th>
<th>Adsorption Energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>4.897297</td>
</tr>
<tr>
<td>C4</td>
<td>4.897277</td>
</tr>
<tr>
<td>C6</td>
<td>4.897311</td>
</tr>
<tr>
<td>C12</td>
<td>4.897346</td>
</tr>
<tr>
<td>B1</td>
<td>4.70065</td>
</tr>
<tr>
<td>B10</td>
<td>4.69786</td>
</tr>
<tr>
<td>B12</td>
<td>4.69770</td>
</tr>
<tr>
<td>B32</td>
<td>4.69623</td>
</tr>
</tbody>
</table>

Figure 4 Total electron density distribution (units: e/Å²) corresponding to the structure of Figure 3. The plane shown is perpendicular to the graphene sheet and contains symmetry axis S indicated in Figure 2.

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