Adsorption of Pt on defective carbon nanotube walls: a DFT approach

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In fuel cells, platinum is used as a catalyst to produce atomic hydrogen[1,2]. In order to utilize carbon nanotubes (CNTs) as the Pt carrier electrodes, a sufficiently high binding energy between Pt and the CNT wall is necessary[3]. Pure CNTs have shown to produce low loading amounts of Pt catalyst particles, which is attributed to the weak adsorption of Pt on the CNT walls[4]. However, Pt adsorption has been improved with defective CNT surfaces[5].

![Figure 1](image-url) Configuration of a Pt atom adsorbed on the wall of a pure, a Stone-Wales and a vacancy site of the (5,5) carbon nanotube.

In present work we have applied density functional theory[6] for studying the adsorption of a single Pt atom on defective single-walled carbon nanotubes (SWCNTs), for a semiconducting (8,0) and a metallic (5,5) SWCNT. Figure 1 shows the most stable configuration for the Pt atom adsorbed on the pure and defected wall of the (5,5) SWCNT. A similar configuration applies to the (8,0) SWCNT. The binding energy is calculated as the difference between the total energies of the adsorbed system and the separate species: $E_b = E_T[\text{CNT}] + E_T[\text{Pt}] - E_T[\text{Pt-CNT}]$. The binding energies and bond distances are summarized in Table 1 for both nanotubes in the configurations from Figure 1. The binding energy on defective SWCNTs is always larger than that on pure SWCNTs. More importantly, the binding energy at vacancy sites is about twice that of any other configuration.

In conclusion, the stronger binding energy at defect sites enhances Pt adsorption on defective SWCNTs. Therefore carbon nanotubes with a high degree of vacancy defects should be most suitable as Pt carrier electrodes in fuel cells.

Table 1. Platinum adsorption energy $E_b$ (in eV) on the (5,5) and (8,0) carbon nanotubes, and the corresponding distance to nearest C atom (in Å).

<table>
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<tr>
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<th>CNT(5,5)</th>
<th>CNT(8,0)</th>
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<tbody>
<tr>
<td>$E_b$</td>
<td>Pt-C</td>
<td>$E_b$</td>
</tr>
<tr>
<td>Pure</td>
<td>2.53</td>
<td>2.07</td>
</tr>
<tr>
<td>Stone-Wales</td>
<td>2.86</td>
<td>2.11</td>
</tr>
<tr>
<td>Vacancy</td>
<td>6.56</td>
<td>1.93</td>
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REFERENCES


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