Graphene Coatings – Probing the Limits of the One Atom Thick Protection Layer

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Supporting information

Details on calculating the energy difference when lifting the reconstruction

For evaluating if a lifting of the reconstruction is favorable, one meets the difficulty that the initial and final configurations to be compared consist of different numbers of atoms. For the unit cell describing rotation 1, which covers an area of 4.73 nm^2, 12 Pt atoms will be in excess when the quasi-hexagonal Pt layer in the initial configuration is transformed into a Pt(100) layer in the final configuration. However, the most stable Pt island obtained contains 16 Pt atoms (1/3 more Pt atoms than available in the unit cell). Therefore the energy of 1/3 extra (1.58 nm^2) graphene on Pt(100) surface, $E(Pt(100)/gr)$, was added to the energy of the final configuration, E(F).

For the initial configurations different approaches were followed. For the cluster initial configuration (I^{cluster}) the energy of 1/3 extra (1.58 nm^2) graphene on hex-reconstructed Pt(100) surface, $E(hex - Pt(100)/gr)$, was added to the energy of the initial configuration, E(I^{cluster}). For the dimer initial configuration it was attempted to have the correct density of dimers on the surface or something close to. For the high coverage, 9 dimers (18 H atoms) were adsorbed

within the unit cell and the energy of the structure was multiplied by 4/3 (increasing the surface area from 4.73 nm^2 to 6.30 nm^2).

Thereby the energy difference starting from the cluster initial configuration was evaluated as:

$$\Delta E_\theta^{cluster} = E(F_\theta) + \frac{1}{3}E(Pt(100)/gr) - E(I_\theta^{cluster}) - \frac{1}{3}E(hex - Pt(100)/gr)$$

and starting from the dimer initial configuration (high coverage) it was evaluated as:

$$\Delta E_{high}^{dimer} = E(F_{high}) + \frac{1}{3}E(Pt(100)/gr) - \frac{4}{3}E(I_{high}^{dimer})$$

All energy differences were normalized to unit area by dividing with 6.30 nm^2. A similar approach was followed for evaluating the energy differences at low and medium coverage on rotation 1 and at high coverage on rotation 2.

For calculating the coverage of H/C atoms on rotation 1, the number of C atoms in the graphene had to be multiplied by 4/3 in order to have the right surface area. The unit cell contains 176 C atoms, and thus the coverage, Θ, was calculated as:

$$\theta = \frac{24}{176 * 4/3} * 100\% = 10.2\%$$

for the high coverage on rotation 1. The low and medium coverage on rotation 1 and the high coverage on rotation 2 were calculated in a similar way.