Substrate-mediated interactions of Pt atoms adsorbed on single-wall carbon nanotubes: Density functional calculations

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Abstract: In this study, we perform density functional calculations to investigate the interplay between single-wall carbon nanotube (SWNT) supports and adsorbed Pt atoms. We found that adsorption of Pt atoms on SWNTs is found to depend heavily on the curvature of SWNTs. The supporting SWNTs mediate and enhance the range of interactions between Pt adatoms. The long-range interactions originate from the structural deformation of the tube and the complex electronic states formed during the adsorption. Furthermore, these SWNT-mediated interactions significantly modify the diffusion barriers of Pt adatoms on the tube surface.

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- The large-scale DFT calculations were carried out using the OpenMX code and using the supercells of 32 conventional unit cells of the (5, 5) SWNT and 16 conventional unit cells of the (10, 0) SWNT. All calculations were performed at the Γ point. Structural optimizations without constraint were carried out for each Pt-Pt distanceThe electron density at a distance of r0 =2.135 far from the nuclear of a hydrogen atom is 10-4 a.u. The binding energy of two hydrogen atoms is in order of 10 meV when their interatomic distance is 2 r0Lau, K.H., (1978) Solid State Commun., 28, p. 757. , 10.1016/0038-1098(78)91339-X
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