

ATOMISTIC SIMULATIONS OF CATALYTIC CARBON NANOTUBES GROWTH

JinJin Wang, John Robertson

Department of Engineering, University of Cambridge, Cambridge CB3 0FA, United Kingdom
jw528@cam.ac.uk

Carbon nanotubes (CNTs) have remained an attractive topic since their discovery in 1991. [1] The interests of their potential applications largely arose from their unusual structural and electronic properties. It is crucial to have a full understanding of the formation mechanisms of the CNTs in order to yield a limited distribution of nanotube chiralities. Besides experiments, the CNTs growth can also be studied theoretically using Density Functional Theory (DFT). [2-4] In this report, we investigate how different catalysts would change the growth of SWNTs.

The SIESTA ab-initio code [5] within the PBE parameterization of the generalized gradient approximation (GGA) was used to calculate the total energy of nanotube caps on different transition metal (Fe, Co, Au, Mo, Ti) surfaces. All the surfaces were built from the (111) surface. We described the valence electrons of C and the metal by a double- ζ and single- ζ polarized basis set, respectively. Caps were relaxed with the metal atoms fixed. The energy of the cap was found by joining two identical caps into a fullerene. Excess energies were corrected for the basis set superposition error.

Our studies of the nucleation stage of the CNTs growths strengthen the idea that selectivity must start during nucleation. [6] Our preliminary results show that for all transition metals the energy of the C-M bonds for the armchair edges are higher than those with zigzag edges by 30% in average; this indicates that the armchair CNTs are more favourable than the zigzag ones. For the same cap, the total energy is also affected by the position of where it was placed. In general, a more stable structure can be achieved when the edge atoms were above the metal bonds. Fig. 1 shows how the structures of the same cap vary depending on their position. However, the relative stability varies according to metal catalysts. From our calculations, Ti offers the most stable structures, while Mo and Co provide a less strong bond with those edge carbon atoms.

References:

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Figures:

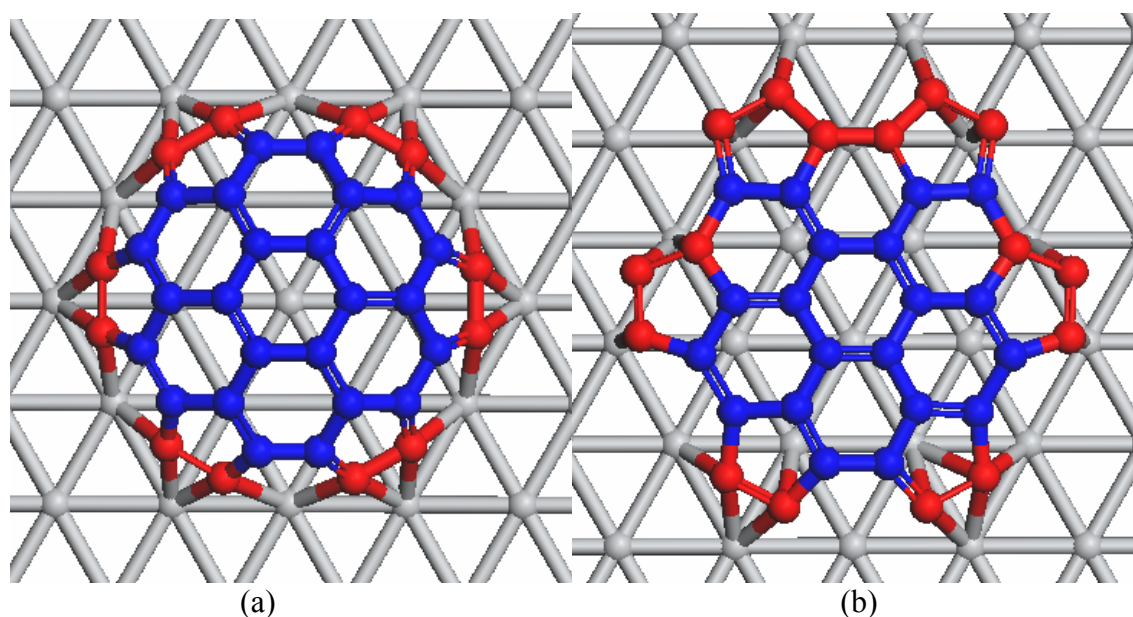


Fig. 1 Relaxed (6, 6) cap on Ti (1 1 1) with the centre hexagon above (a) Ti atom (b) Ti hole site