**The Nature of the Carbon Nanotube – Catalyst Interface during Chemical Vapour Deposition Growth**

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Carbon nanotubes (CNTs) are single layers of carbon atoms rolled into cylinders. While only ~1 nanometer in diameter, CNTs can be up to millimetres or centimetres in length. CNTs therefore consist of billions of carbon atoms arranged in a perfect hexagonal lattice. CNTs are “grown” from a metal catalyst surface via a process known as chemical vapour deposition, which decomposes hydrocarbons and rearranges their carbon atoms into CNTs. This growth process is thus a unique form of crystal growth – the precise arrangement of the billions of carbon atoms in a CNT is ultimately controlled by a growth interface that is only ~1 nanometer wide and consists of only a handful of atoms (Figure 1). Despite the maturity of the CNT growth field, we continue to discover many fundamental aspects regarding this growth interface that are key to achieving chirality-controlled CNT growth. For instance, the importance of CNT edge configurational entropy in explaining the growth of chiral tubes [1] and the existence of CNT edge faceting during growth [2]. In this talk I will discuss how the temperature and catalyst metal influences these and other phenomena related to the CNT growth interface, and how they relate to strategies for chirality-controlled CNT growth with solid and liquid phase catalyst nanoparticles. I will also show that the extent of charge transfer between armchair and zigzag atoms in the CNT edge and the catalyst surface are different and discuss how this phenomenon is influenced by applied electric fields, relevant to the recently-reported ‘electrotwisting’ strategies for controlling CNT metallicity *in situ* during growth [3].



**Figure 1.** Relative energies (eV) of CNT-catalyst interfaces as a function of the CNT edge structure for liquid phase Ni (left) and Co (right) catalysts. In contrast to solid-phase catalysts, the preferred edge structure at the interface is catalyst dependent.

**References**

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