Understanding Catalytic Carbon Nanotube Growth Through Density Functional Theory Calculations

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To utilize the unperturbed inherent electrical properties of carbon nanotubes it's necessary to produce the single-walled type (SWNTs) of specific diameter and chirality (index). Catalytic CVD growth has scored tremendous advances in controlling the diameter and, using template catalysts and seed-molecules, product with one single index. Only certain metals act as catalyst and we have shown through density functional theory (DFT) computations that specific for CNT growth is its ability to stabilize the growing end and to prevent it from closing.

Thus the catalytic metal - CNT binding strength follows a 'Goldilocks criterion' where the tube-end cannot bind too weak or too strong to the metal. Our recent DFT work show which of all 1st, 2nd and 3rd row transition metals are in this zone, and could be used as catalysts in CVD. We also show how metals outside the zone (non-catalytic) can be combined to work as catalysts. In addition, we will present work where we have compared experimental product with SWNT stability from DFT, for which we surprisingly find strong correlation. We will shed light on how armchair and zigzag ends form bonds that are individually equally strong, but collectively show huge stability differences.