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Exploration of Nanotube Structure Selectivity Using Bimetallic Catalysts[1]

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Achieving selectivity for nanotube chirality is one of the holy grails for single-walled carbon nanotube research. One approach we are following is based on the ability to engineer the size and state of the initiating metal particle to constrain the type of cap formed. The chirality/structure of a nanotube is controlled by carbon cap formation on the metal particle during the nucleation step. It has been proposed that varying the carbon-metal catalyst binding energy could help lead to structure selectivity. One reason theoretically proposed for the favoring of armchair nanotubes, for example, is the proximity of low energy binding locations for two carbon atoms. Thus blocking sites or perturbing the binding energy on adjacent sites could in theory affect the structure of the carbon cap formed in the nucleation step. Our goal is to demonstrate structure selectivity in the growth of single wall carbon nanotubes (SWNT) using a bimetallic catalyst. The catalyst used was a bimetallic CoCr-MCM 41 and the effect of different molecular ratios between the two metals on the SWNT diameter distribution was studied. We have found that by adding Cr to the Co-MCM 41 monometallic catalyst the diameter distribution shifted in a systematic manner correlated to the development of a bimetallic phase as characterized by X-Ray absorption spectroscopy (XAS). We have also found that the shift is accompanied by suppression of metallic SWNT, particularly those with diameter over 0.9 nm. We are also currently exploring the possibility of a further narrowing of the distribution by lowering the reaction temperatures.

[1] In collaboration with Codruta Zoican, Yale University.