Towards chirality-control: Catalyst-free growth of single-wall carbon nanotubes on SiOy nanoparticles

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Chirality control (CC) during CNT growth becomes increasingly important along with the tremendous

success of CNT in so many applications. The metallic catalysts which have demonstrated their important

role in CC have its unavoidable limitations such as pollution. Therefore non-metallic catalyst becomes appealing. The chirality control of catalyst-free growth of single-wall carbon nanotubes on SiOy nanoparticles have been demonstrated to be possible. Some vague experimental demonstrations from the literature seem insufficient. In this talk, we show how we understand the mechanism behind it by combining ab initio molecular dynamics simulations and pair distribution function(PDF) analysis.