21COE Programme: Mechanical Systems Innovation Open Seminar

21COE Programme: Mechanical System Innovation 11th Open Seminar 2005 will be held as follows. Any participants will be welcome. People from Materials, Electrical engineering and Physics fields may also be interested in the topic.

Invited Speaker: Dr. Stephan Irle (Cherry Emerson Center for Scientific Computation, Emory University)

Title: Nucleation and growth of SWNTs studied by QM/MD simulations

Date & Time: 18 October 2005 (Tuesday), 14:00~15:30

Place: The University of Tokyo, Engineering Building No.8, 2nd Floor, Conference Room No.226

Abstract: Achieving control over number of carbon nanotube (CNT) layers, chirality and diameter distributions at the time of synthesis is the holy grail of carbon nanotube research, since it would allow to eliminate time consuming, expensive, and potentially destructive purification steps. The parameters governing CNT structural characteristics must be effective at the very early stages of CNT nucleation, therefore it is very important to gain atomic level understanding of the catalyst/carbon chemistry involved in CNT nucleation and further growth. Unfortunately, the time scale for these reaction steps is inaccessible to experiment. Using quantum chemical molecular dynamics (QM/MD) simulations of high-temperature carbon plasma, we have recently discovered the "shrinking new giant" road of fullerene formation using density functional tight binding (DFTB) quantum chemical potential. We are presenting in this talk QM/MD simulations for iron catalyzed single-walled carbon nanotube SWNT nucleation and growth. Isokinetic trajectories at 1500 K to 3000 K show that divalent Fe increases the number of coordination partners with carbon and/or Fe, depending on the Fe concentration. Fe/C interactions weaken the tube sidewall due to electron transfer from Fe into antibonding carbon orbitals, and C2 addition occurs mainly in an Fe-C2-Fe bridge addition mechanism, while growth of polyyne chains characteristic for fullerene formation is suppressed in the presence of Fe on the rims of the growing SWNT. Our findings are the first direct quantum chemical evidence for the importance of intermetallic interactions and therefore the validity of the metal-particle model.

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