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The initial stages of nitrogen-doped single-walled carbon nanotube growth

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We have studied the mechanism of the initial stages of nitrogen-doped single-walled carbon nanotube growth illustrated for the case of a floating catalyst chemical vapor deposition system, which uses carbon monoxide (CO) and ammonia (NH3) as precursors and iron as a catalyst [1,2]. First, we performed first-principles electronic-structure calculations, fully incorporating the effects of spin polarization and magnetic moments, to investigate the bonding and chemistry of CO, NH3, and their fragments on a model Fe55 icosahedral cluster [3]. A possible dissociation path for NH3 to atomic nitrogen and hydrogen was identified, with a reaction barrier consistent with an experimentally determined value we measured by tandem infrared and mass spectrometry. Both C–C and C–N bond formation reactions were found to while a parasitic reaction of HCN formation had a barrier of over 1 eV. Furthermore, we studied the dynamics of carbon and nitrogen atoms on the Fe55 nanoparticle by means of molecular dynamics simulations at the density-functional tight-binding level [4]. A time range of at most 0.4 ns was covered in the molecular dynamics simulations and different degrees of adatom coverage were considered. Nitrogen and carbon atoms expressed different dynamics. Adsorbed monomers and large fragments were rather immobile whereas dimers and trimers move fast. Nitrogen-containing fragments were less strongly bound to the iron cluster and therefore more mobile than carbon-only fragments with equal amount of atoms. On the iron nanoparticle surface, five-membered rings were formed first and then six-membered rings.

[1] T. Susi, Z. Zhu, G. Ruiz-Soria et al., Physics Status Solidi B 247 (2010) 2726.
[2] T. Susi, A. Kaskela, Z. Zhu et al., Chemistry of Materials 23 (2011) 2201.
[3] T. Susi, G. Lanzani, A.G. Nasibulin et al., Phys. Chem. Chem. Phys. 13 (2011) 11303.
[4] S. Taubert and K. Laasonen, J. Phys. Chem. C 116 (2012) 18538.

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