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Surface diffusion of a carbon adatom on charged SWCNT[1]
LONGTAO HAN, PREDRAG KRSTIC, State Univ of NY- Stony Brook, IGOR KAGANOVICH, Princeton Plasma Physics Laboratory — Diffusion of a carbon adatom on SWCNT could be a mechanism for a CNT growth in a volume plasma, supplementing its growth from a transition metal catalyst nanoparticle. However, being embedded in plasma, the nanotube can charge by the plasma particles irradiation, in particular by electrons. Using Density Functional Theory, Nudged Elastic Band and Kinetic Monte Carlo methods we find (1) equilibrium sites, (2) adsorption energies, (3) potential barriers, (4) vibrational frequencies and (5) most probable pathways for diffusion of the adatom on external surfaces of SWCNTs of (5,5), (10,0) and (10,5) chirality, as function of its charge. The metal (5,5) SWCNT can support a fast diffusion of the carbon adatom, which is accelerated by the presence of the SWCNT negative charge. Reduced model of SWCNT growth is proposed.

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