James M. Hill et al., Madridge J Nanotechnol Nanosci. 2018
http://dx.doi.org/10.18689/2638-2075.a3.004

3rd International
Nanotechnology Conference & Expo
May 7-9, 2018 Rome, Italy

Continuous Approximation for Interaction Energy of Adamantane Encapsulated Inside Carbon Nanotubes

James M. Hill[2]*, Duangkamon Baowan[1] and **Wolfgang Bacsa[3]**
[1]Department of Mathematics, Faculty of Science, Mahidol University, Thailand; Centre of Excellence in Mathematics, Thailand
[2]School of Information Technology & Mathematical Sciences, University of South Australia, Australia
[3]CEMES-CNRS and University of Toulouse, France

Linear forms of crystalline diamond constitute a new one-dimensional nanomaterial. They assemble within carbon nanotubes which serve as a template and by taking diamondoids as building blocks. Template synthesis of linear chain nanodiamonds have been considered recently using diamantine polymers. The smallest building block of diamond is adamantane, which is the smallest unit with a diamond lattice. The interaction energy for two adjacent adamantane molecules and that of adamantane molecules encapsulated inside carbon nanotubes are investigated. The Lennard-Jones potential and the continuous approximation are utilized to derive analytical expressions for these interaction energies from a highly simplified model. The derived equilibrium distance is found to be within 3% of density functional calculations and an equilibrium distance of 3.281 Angstroms between two adamantane molecules is determined. The smallest carbon nanotube radius b0 that can encapsulate the adamantine molecule and the radius of the tube bmax that gives the maximum suction energy, are calculated to depend linearly on the adamantane radius. For larger diameter tubes, the off axis position is predicted, and the equilibrium distance between the molecule and the tube wall is found to be close to the interlayer spacing in graphene.

Keywords: Adamantane, carbon nanotube, Lennard-Jones potential, interaction energy.