ENGINEERING TH EBAND STRUCTURE O FDECACHLOROFULLERENE[50] CARBON NANOTUBE PEAPODS.

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We use ab initio density functional theory to calculate the structural and electronic properties of decachlorofullerene[50], C50Cl10, carbon nanotube peapods (CNPs).The inhomogenous charge distribution over the C50Cl10 molecule, where the covalently bonded chlorine atoms for maring of negative charge round the rim of the wheel shaped molecule, creates new energetic and electronic characteristics in the CNP due to the electrostatic interaction between the carbon nanotube (CNT) walls and chlorine atoms. One such effect is to induce a splitting of the CNT mini-bands at the X point of the folded CNT which is an extrafeature to appear along side the hybridisation of the CNT and C50Cl10 bands near the HOMO step edge. By exploiting the new degrees of control over the CNP geometry introduced by the electrostatic characteristics we demonstrate a method of engineering the band structures by ordering the C50Cl10 inter-molecule separation within the CNP which results in dramatic changes to the electron transport characteristics through the CNT walls.