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Synthesis and Electronic Properties of Silicon-Nitrogen Hetero-doped Single Walled Carbon Nanotubes MARTHA AUDIFFRED, Universidad de Guanajuato, Mexico, ANA LAURA ELIAS, HUMBERTO R. GUTIERREZ, PSU, FLORENTINO LOPEZ-URIAS, IPICyT, HUMBERTO TERRONES, PSU, MAURICIO TERRONES, PSU, Shinshu University, GABRIEL MERINO, Universidad de Guanajuato, Mexico — We investigated the stability and electronic properties of hetero-doped carbon nanotubes using first-principles density functional theory. Silicon, silicon-nitrogen, and silicon-oxygen were incorporated within the lattice of different types of single-walled carbon nanotubes. The structural stability, electronic density of states, doping energy, band structure, HOMO and LUMO were analyzed. When silicon and nitrogen are bonded and inserted in the nanotube lattice, non-dispersive bands appear around the Fermi level. The Nitrogen arranged in a pyridine-like fashion together with a silicon atom placed inside the vacancy was also studied. The latter configuration becomes more stable than the substitutional nitrogen embedded in the (9,0) and (5,5) nanotubes. We have also succeeded in the synthesis of Si and SiN-doped single-walled carbon nanotubes (CSixNy -SWNTs) by chemical vapor deposition. We carried out Raman spectroscopy, high-resolution electron microscopy, electron energy loss spectroscopy, energy-dispersive X-Ray spectroscopy, Auger spectroscopy and X-Ray photoelectron spectroscopy, in order to identify the presence of both dopants within the nanotube lattice.

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