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Electronic band structure of Hydrazine-water doped Single-Walled Carbon Nanotubes as n-Type Semiconductor

Thursday, May 21, 2015 8:00 AM (3 hours)

We have studied the electronic band structure of single-walled carbon nanotubes (SWCNTs), (8,0) 3 primitive cells 96 carbon (C) atoms doped with hydrazine (N_2H_4) and water (H_2O). Van der Waals corrected density functional theory calculations using plane wave approach with periodic boundary conditions were carried out for the adsorption of the intermolecular interaction. The results indicate that hydrazine physisorbs to the surface of SWCNTs and carbon atoms still retains the formal sp2 hybridization. Furthermore, the electronic structures and Bader charge analysis of the considered complex reveal the band gap of intrinsic semiconductor changed from 0.6 to 0.4 eV, as n-type semiconductor. The configuration of hydrazine and water, hydrogen bonding network supported, are important key to occur donor state in physisorption doping process.

Primary author: Dr KOMIN, sittipong (Department of Physics, Faculty of Science, Ubonratchathani University, Ubon Ratchathani 34190, Thailand)

Co-authors: PRACHAMON, Wutthisak (School of Physics, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand); Prof. LIMPIJUMNONG, sukit (School of Physics, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand)

Presenter: PRACHAMON, Wutthisak (School of Physics, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand)

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