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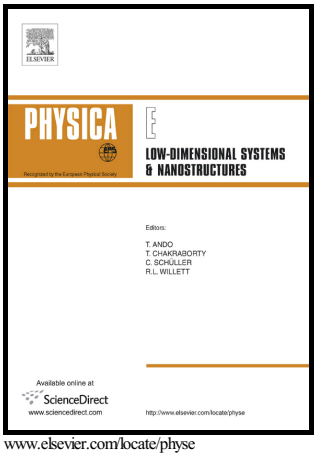


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# Co-doping as a tool for tuning the optical properties of singlewalled carbon nanotubes: A first principles study

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## Abstract:

This paper presents a first principles study on the effect of co-doping on various optical spectra of a zigzag single-walled carbon nanotube (SWCNT). Optical spectra of a pristine SWCNT , SWCNT co-doped with Aluminum (Al) & Phosphorus (P) and another one co-doped with Al, P and Nitrogen (N) have been calculated using density functional theory (DFT).The theory has been implemented using the Cambridge sequential total energy package (CASTEP) code available as a userfriendly module with the software 'Material Studio'. Polarized and unpolarized light as well as light through polycrystalline media have been considered. The dependence of various spectra on the status of incident light presents a clear evidence of anisotropicity in the optical properties. Analysis of the simulated spectra involves calculation and comparison of different optical properties like dielectric function, reflectivity, refractive index, conductivity and loss function for the pristine and co-doped SWCNTs. Noticeable variations are observed in the optical properties on simultaneously doping the SWCNT with Al and P and then further introducing N atom into the structure so that it can be concluded that co-doping (simultaneous doping with different combinations of dopants) can be evolved as a novel and effective tool for tailoring the optical properties of SWCNTs as per the requirements while