**Luminescent properties of defects on Single-Walled Carbon Nanotubes**

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Semiconducting single-walled carbon nanotubes (SWCNTs) are appealing candidates for applications such as single-photon emission and high-contrast bio-imaging. Incorporating $sp^3$ quantum defects in the sidewalls of SWCNTs through chemical reaction is an excellent route to predictably modify nanotubes optical, electronic structures and develop advanced optoelectronic functionality. In aryl functionalized SWCNTs, the binding configurations of the aryl group define the energies of the emitting photons[1]. Here, we explore protocol to control chemical binding configurations of quantum defects on SWCNTs also referred as organic color centers through the photoexcited states. Simulations were performed to optimize the N-methyl-di-oxy-pyrrole functionalized SWCNTs (11,0) and (10,0) at three different ortho binding configurations (o++, o+ and o-). Density functional theory (DFT) calculations were performed using VASP with the generalized gradient approximation (GGA) Perdew−Burke−Ernzerhof (PBE) functional in a plane-wave basis set along with projector augmented-wave (PAW) pseudopotentials. For approximate evaluation of optical spectra, the oscillator strengths for HOMO-LUMO transitions were obtained by adopting independent orbital approximations. Non-adiabatic calculations are performed to allow dissipation of energy from electronic to nuclear degree of freedom to explore non-radiative relaxation of excited states[2]. The outcome of controlled chemical functionalization in the SWCNTs activates the red-shifted photoluminescence with longer lifetimes and higher photoluminescence yield. We correlate our results with different experimental studies to better understand the opto-electronic behavior of defect-states of functionalized CNTs[1]. These findings impact practical applications of a variety of nanotubes as quantum light sources for quantum information technologies that can be expanded to controlled chemical functionalization of any nanomaterials.

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References

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