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Investigation of Poly(2,5)-benzimidazole (ABPBI)-Carbon Nanotube Composites for LEO Applications: An Integrated Computational and Experimental Study

This study explores the potential of an ABPBI–carbon nanotube composite as a candidate for space coating applications in Low Earth Orbit (LEO), using a combined computational and experimental approach. The goal is to assess how the composite's structural, electronic and optical properties respond to the demanding conditions of the space environment.

Density functional theory (DFT) as implemented in the CASTEP program was employed to construct and analyse a single-walled carbon nanotube (SWCNT) supercell with an adsorbed ABPBI monomer. Geometry optimisation, density of states (DOS), band structure (BS) and absorption spectrum analyses were conducted. Results showed significant π–π stacking interactions between the polymer and nanotube, charge redistribution and a notable decrease in the bandgap. These changes suggest improved electrical conductivity and enhanced absorption in the UV region.

Complementing the simulations, experimental studies were conducted on multi-walled carbon nanotube (MWCNT) reinforced ABPBI films. Optical characterisation using ultraviolet–visible (UV–Vis) spectroscopy and photoluminescence (PL) measurements revealed a consistent blue shift in the absorption peaks and noticeable changes in fluorescence intensity with increasing carbon nanotube (CNT) concentration. These effects indicate strong electronic interactions between ABPBI and the nanotubes. The widened Stokes shift observed in the PL results further supports improved charge separation and emission behaviour.

Overall, the experimental findings align well with the computational predictions, confirming that nanotube incorporation alters the electronic and optical response of ABPBI in a controlled and beneficial way. While the composite demonstrates properties—such as strong CNT–polymer coupling—further studies are recommended to evaluate its thermal performance and mechanical resilience under extended LEO exposure. The strong agreement between computational and experimental work in this study lays a foundation for further exploring the durability of ABPBI composites in the volatile environment found in LEO.

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