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Probing non-covalent interactions within π - π stacking assembly by EPR Spectroscopy

ABSTRACT

π - π stacking interactions play a fundamental importance for the further development of supramolecular chemistry, materials science and tuning and prediction of the crystal structures by controlling self-assembly and molecular recognition. However, the nature of π - π stacking interactions remains unclear. In order to elucidate the insight, Electron Paramagnetic Resonance (EPR) measurement was carried out to investigate the insight of the interactions within π - π stacking assembly. Carbon nanotubes (CNTs) exhibit extended π electron clouds, while the phenyl rings in the polyimide (PI) show localized π electrons. Since the introduction of CNT into aromatic PIs is accompanied by the recombination or movement of unpaired electron, EPR should be a powerful method for probing the paramagnetic products of the introduction of CNT into polyimides process. EPR measurement results indicate that the resonance line parameters of $g = 2.003 \pm 0.001$ and peak-to-peak linewidth $l_{pp} = 7 \pm 1$ G is generated for the polyimide films. Polyimide samples with CNT have a second resonance at slightly larger magnetic field values and has a $g = 2.008 \pm 0.001$. Neat PI displays a symmetrical and relatively higher intensity EPR signal in comparison to CNT/PI nanocomposites. Intensity ratio of PI central resonance aroused by aromatic group of PI between the neat PI and CNT/PI nanocomposites indicating that these paramagnetic centers are influenced by the electronic structure of CNT surface. Compared with neat PI nanocomposites, CNT/PI nanocomposites show almost less than one third of intensity at the central PI resonance, which indicates a decreased generation of unpaired electrons originated from imide group in the presence of CNT. The findings are significant to elucidate the nature of non-covalent interactions within π - π stacking assembly.

Keywords: Non-covalent interactions, π - π stacking, EPR, Carbon nanotubes, Polyimides

BIOGRAPHY

I hold PhD at 2013 from Harbin Institute of Technology (one of top nine C9 League of Chinese Universities). In 2016, I was affiliated with the school of mathematics and physics of University of Freiburg as a Post doctor; Currently, I am working at Liaoning petrochemical University as a professor. Research interests focus at non-covalent interactions, nanomaterial construction, polymer science and composite materials