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Molecular dynamics studies of the transfer of protons in multi-walled carbon nanotube poly(2,5)benzimidazole composites

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In Low Earth Orbit (LEO), some dangers spacecraft electronics are subjected to are high energy protons [1]. Their energies range from a few MeV to GeV [2]. The current shielding employed by spacecraft (consisting mainly of satellites) is insufficient in protecting internal electronics [3]. In the past, and still, an extensively researched avenue is to employ polymers and composites as a radiation shielding mechanism [4]. This is due to their desirable lightweight and excellent mechanical properties [4]. One such polymer meeting this criterion is Poly(2,5)benzimidazole (ABPBI) [5] and ABPBI with multi-walled carbon nanotube (MWCNT) enhancement. Its interactions with energetic protons were investigated using molecular dynamics (MD) [6]. The mean square displacement (MSD) and radial distribution function (RDF) [7] reported in this work aid in seeing how these interactions change due to different weight percentages (1%, 3%, and 5% load of MWCNT). A Perl script was implemented to quantify and monitor variations in the paths available in the samples for proton hopping. These methods help indicate the most likely path the energetic proton moved through [7]. This investigation considers the efficacy of using ABPBI, and its composites, as a proton shielding material for LEO spacecraft applications and further considers changes due to adding carbon nanotubes.

References

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Primary authors: VAN NIEKERK, Salomon (NWU); Dr SQUARE, Lynndle (North West University)

Presenter: VAN NIEKERK, Salomon (NWU)

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