

Abstract Submitted
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A Systematic Study of Noncovalent Interactions Between Polymers and Carbon Nanotubes via Molecular Dynamics Simulations

MELISSA PASQUINELLI, SYAMAL TALLURY, Fiber and Polymer Science, North Carolina State University — Molecular dynamics simulations were used to study the noncovalent interactions between a zig-zag single-walled carbon nanotube (SWCNT) and polymer chains with varying degrees of saturation, aromaticity, and aliphaticity. The simulations indicate that polymers with both flexible and rigid backbones tend to wrap around the SWCNT, although in different conformations. Flexible backbones wrap in random conformations, which are dependent upon the aliphatic lengths along the backbone and the presence of chemical groups like carbonyls. Polymers with unsaturation along the backbones tend to have more distinct wrapping conformations, as did polyamides with large alkane portions in the monomer unit such as nylon-12. Polymers with bulky and aromatic side groups such as polymethylmethacrylate (PMMA) and polystyrene (PS) prefer intrachain interactions rather than wrap the SWCNT, although PS showed some pi-pi interactions with the SWCNT. Other trends and the correlation of the physical chemical features to the properties of nanocomposites will be discussed.

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