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Stabilizing Interactions in SWNT – Polypeptide Nanocomposites
KRISTOPHER WISE, CHEOL PARK, National Institute of Aerospace, PETER LILLEHEI, EMILIE SIOCHI, JOYCELYN HARRISON, NASA Langley Research Center — This contribution describes the computational component of a combined experimental and modeling study of nanocomposites consisting of single wall carbon nanotubes (SWNTs) dispersed in synthetic polypeptides. Our experimental results show that these composites possess an attractive suite of mechanical properties including increased modulus, strength, and elongation at break. In addition, the composites exhibit high, isotropic electrical conductivity and improved dielectric properties. Molecular dynamics simulations reveals that a number of stabilizing interactions are operative spanning several length scales. At the atomic level van der Waals bonding dominates. At larger length scales electrostatic interactions between antiparallel aligned α helical peptides promote the formation of bundles containing SWNTs in the centers.

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