

Abstract Submitted  
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**Enhancing Polymer-Fullerene Miscibility Through Enthalpic Interactions** KATIE CAMPBELL, DAVID BUCKNALL, YONATHAN THIO, HASKELL BECKHAM, UWE BUNZ, ADAM HANNON, ANDREW ZAPPAS, BILGE HATIBOGLU, Georgia Institute of Technology, MICHAEL KEMPF, Universität Karlsruhe — Using both theoretical and experimental methods, the use of functional groups in controlling the miscibility between various polymers and fullerenes has been investigated. Molecular dynamics simulations with unmodified C<sub>60</sub> and C<sub>60</sub> dimers indicated that the number and connectivity of phenyl rings as functional groups, polymer backbone spacing, and aromaticity are all factors in fullerene miscibility. To distinguish between entropic and enthalpic factors, UV-visible spectroscopy was used to determine fullerene solubility with a variety of solvents and to also determine association constants with solvents and polymers. A distinct time dependency for complex formation with many of the fullerene-organic materials investigated was observed as evidenced by a change in solution color with time. Stern-Volmer approximations and fluorescence quenching were used to examine the association of C<sub>60</sub> with a series of poly(*para*-phenylene ethynylene)s, cyclic polystyrene (PS), and linear PS. The fluorescence quenching of these materials by C<sub>60</sub> indicates an association between C<sub>60</sub> and the polymer. WAXS studies have shown the formation of C<sub>60</sub> aggregates in PS at concentrations of C<sub>60</sub> as low as 1 wt%.

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