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Computations Related to Nanoparticle Characterization and Nanocomposite Property Estimation FERNANDO VARGAS-LARA, NIST/Wesleyan, AHMED HASSAN, EDWARD GARBOCZI, JACK F. DOUGLAS, NIST — The macroscopic properties of high-performance bulk polymer composite materials derive from the properties of the microscopic building block component particles, the polymer matrix in which they are placed, and the state of particle dispersion. The rational design of new materials then requires the characterization of the polymer matrix and the individual particles, as well as an understanding of how particle properties change as a function of spatial dispersion and particle size polydispersity and shape fluctuations. To systematically explore this multi-dimensional parameter space, we combine molecular dynamic simulations, numerical path-integrations (ZENO) and finite element calculations (COMSOL). As a specific illustration of this computational path, we calculate the electric and magnetic polarizability tensor of carbon nanotubes and graphene sheets having complex morphologies. Knowing these basic particle properties, one then can estimate electromagnetic properties of nanocomposites made with these particles, i.e., conductivity

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