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Ab Initio Calculations for the Optical Properties of Self-Assembled Nanostructures. IGOR VASILIEV, New Mexico State University — Polymeric photonic materials have generated considerable interest in recent years. The dispersion of carbon nanotubes within emissive polymers increases the efficiency of radiative recombination in these materials. The light output can be further enhanced by assembling luminescent molecules on the surface of nanotubes. This study analyzes the interaction of carboxylated nanotubes and molecules of phenosafranin. The geometries, binding energies, and optical absorption spectra of the modeled nanostructures are calculated in the framework of first-principles density-functional and time-dependent density-functional methods. The computed shift in the optical absorption of phenosafranin is consistent with experimental observations and suggests the formation of charge-transfer complexes between phenosafranin and nanotubes.

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