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Study on Nanoparticles in the Photoactive Layer in Photovoltaic Cells Using Chemical and Computational Analysis KYUMIN KIM, CRG-NJ — The current research on organic solar cells has discovered that there are many advantages regarding the use of these solar cells. Organic, polymer-based solar cells, also commonly referred as OSCs, have been found to be a new and better alternatives to inorganic cells in several ways. In this paper, Density Functional Theory (DFT) and calculations were used to study electronic properties of the nanoparticles in the photoactive layer in a solar cell. Various fullerene derivatives including P3HT:PCBM complex were modeled using a molecular editing program to define the efficiencies of the nanoparticle compounds. Three factors, such as thermodynamic stability, dipole moment, and electrostatic potential map, were considered. Relative angular orientation between the two molecules was also considered in finding the stability and the total energy of the P3HT:PCBM complex. The DFT calculations and quantum physical method were used to characterize the electronic properties of those configurations. Fullerene complexes that were optimized in a relatively short period of time were also predicted to be more thermodynamically stable, as short optimization times generally equate to spontaneous converging.

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