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Study on the Active Optical Layers in the Organic Solar Cell to Improve Electricity Using Physical and Computational Analysis CHRIS LEE, St. Marks School, RICHARD KYUNG, Choice Research Group — Solar cell is a photovoltaic cell which produces electricity in the photoactive layer from sunlight by the photovoltaic effect. Many conductive organic polymers can be used in the photoactive layer to increase the efficiency of light absorption and charge the solar cell. In this paper, optical properties of fullerene derivatives, such as optimized energy(kJ/mol), dipole moment(debye) and electro-potential map were determined in the assessment of efficiency of the solar energy. Also variations of the functional group on the fullerenes were considered to check those dependencies on solar energy output. As electron acceptors in the photoactive layer, various types of organic compounds including PCBM, a fullerene derivative [6,6]-phenyl-C61-butyric acid methyl ester, were tested in the present organic solar cell simulations. Computational editing programs have been used in an effort to discover the optimal method and to compute the measurements of stability of the organic nanoparticles used in the solar cell. To determine optimization energy and electrical activity, an auto optimize tool was used for each fullerene derivative in this project. Also, the Universal Force Field (UFF) option was selected and applied to all fullerene derivatives modeled in this research.

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