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Optical and Thermodynamic Analysis of Organic Solar Cells Using Physical and Computational Simulations WOONG JAE BAEK, University of Illinois–Urbana-Champaign, ANDREW KYUNG, Northern Valley Regional HS — An organic solar cell is a type of photovoltaic cell which produces electricity from sunlight by the photovoltaic effect. Conductive organic polymers are used for light absorption and charge the cell. Optical properties and constants of isotropic thin P3HT:PC61BM film systems, such as refractive index, relative permittivity (dielectric constants), wavelength were considered in the calculations of solar energy. Also the geometrical variations such as thickness and width, and material properties were considered to check those dependencies. Poly(3-hexylthiophene) (P3HT) which is a hydrophobic and well stacking semiconducting polymer was used as an electron donator in the current organic electronics simulations. As an electron acceptor, PCBM, a fullerene derivative [6,6]-phenyl-C61-butyric acid methyl ester, was used in conjunction with the electron donor materials P3HT. The computational programs such as Avogadro and Chemcraft have been used in an effort to discover the optimal method and to compute the measurements of stability of the solar cell. The Auto Optimize Tool was used for each and every fullerene derivative modeled in this project to determine its optimization energy. The Universal Force Field (UFF) option was selected for all fullerene derivatives modeled.

Richard Kyung
Choice Research Group

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