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Stability Analysis of Nanoscaled Molecules Used in Organic Solar Cells Using Computational Simulations HYUN KI CHO, RICHARD KYUNG, Choice Research Group — Organic solar cells are crucial in the production of solar cells, and they can result in many advantages such as the relatively high absorption coefficient and cheaper production cost compared to inorganic solid-state semiconductors. But the stability problems due to a few factors such as heating and mechanical stress still remain a great challenge, although the power conversion efficiencies have increased over the years. Since the mechanism of organic solar cells is fundamentally different from that of silicon based inorganic semiconductor based technologies, understanding the material and chemical properties of organic solar cells at the nano scaled molecular level is crucial. The purpose of this project is to study the fullerenes potential to be used in solar cell semiconductors. Avogadro was used to model the fullerenes when connected to functional groups. 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.

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