

Anthropomorphic Molecules as the New Candidates for Photovoltaic Applications

Foroogh Arkan¹ and Mohammad Izadyar¹

¹Ferdowsi University of Mashhad

March 30, 2022

Abstract

Here, photovoltaic behaviors of the human-shaped molecules named Nanokid and Nanoathlete (monomeric forms) and Nanoputain dimer1 and Nanoputain dimer2 (hetero-dimers) based on the quantum chemistry were investigated. For all studied anthropomorphic molecules, tuning the electrophilicity decreases the energy barrier of the electron injection. Nanokid and Nanoathlete have greater activity against solar light, which shows more favorable photovoltaic parameters. Although Nanoputain dimers represent better charge transfer indices and intramolecular charge transfer, they have low oscillating strength. The maximum peaks of the current and efficiency in different absorption wavelengths are originated from the increase in the light-harvesting efficiency and decrease in the energy barrier of the electron injection. Finally, Nanokid and Nanoathlete are proposed as better candidates to be used in the photovoltaic cells.

Hosted file

paper2-j QUANTUM CHEM..-me-.docx available at <https://authorea.com/users/342312/articles/562077-anthropomorphic-molecules-as-the-new-candidates-for-photovoltaic-applications>