

## New KuQuinone for solar cells applications

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We have investigated the structural, morphological and optical properties of dibenzofluorene derivative, which is part of the new sub-class of dibenzofluorenes, due to its existence as a zwitterion, in contrast to other KuQuinones. Microstructural and morphological characterization data, as well as powder X-ray diffraction study, confirm the amorphism of dibenzofluorene derivative in the present form. The  $E_g$  value calculated from the absorption and transmission spectra of thin films indicates the ease of the electrons transporting from the HOMO level to the LUMO level during light absorption. The optimization of the dibenzofluorene derivative was performed using density functional theory (DFT) by the M06-2X/cc-pVTZ + PCM (CH<sub>3</sub>CN) method. The UV spectra were calculated using CAM-B3LYP/cc-pVTZ and W97X/cc-pVTZ + PCM (CH<sub>3</sub>CN) methods. Our theoretical results confirm and explain the obtained experimental data. As a result, this material is expected to be applied as a light harvester thin-film and an optoelectronic design for further applications.

### Topics

Session D. Biomedical optics and sensors technology

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