

Article

# Density Functional Theory-Based Molecular Modeling: Verification of Decisive Roles of Van Der Waals Aggregation of Triiodide Ions for Effective Electron Transfer in Wet-Type N3-Dye-Sensitized Solar Cells

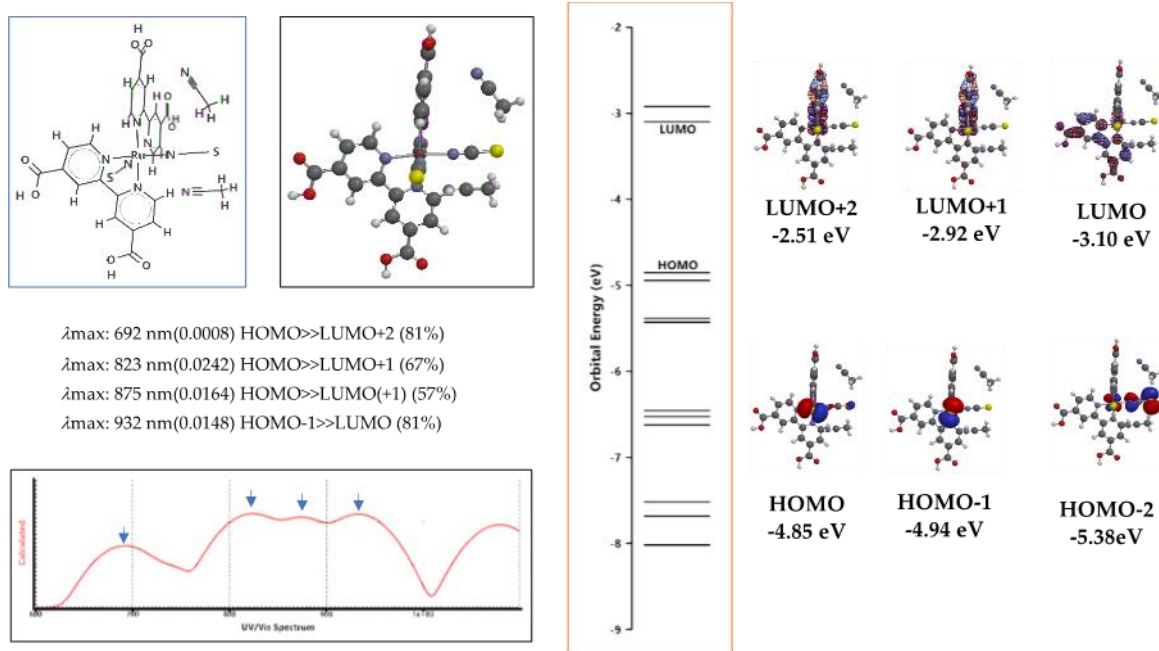
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**Supplementary:** Energy structure of vdW-aggregate of N3 with acetonitrile (AN) of N3 and (AN)<sub>2</sub>: UV/Vis spectrum and surface electron energy structure.