

Electrolyte-Free Dye-Sensitized Solar Cell with High Open Circuit Voltage Using a Bifunctional Ferrocene-Based Cyanovinyl Molecule as Dye and Redox Couple

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Integrating additional functionalities to a functional material and applying them in useful devices are the universal strategy to design multifunctional materials. Ferrocene based organometallic compounds have gained lots of research attention because of their interesting properties related to redox switching, optical non-linearity, electronic communication, molecular receptor, sensors etc. The intrinsic redox property of the ferrocenyl fragment has made them a potential candidate in dye sensitized solar cells (DSSC); mostly as a redox electrolyte to improve the device efficiency. In this communication we have reported the functionalization of ferrocenyl moieties with cyanovinyl system using a unique solid state synthetic method which led to the formation of donor-acceptor type compounds with wide absorption in the visible region. DSSC study using the ferrocenyl cyanovinyl compound as dye with an electrolyte-free fabrication system showed an unprecedented open-circuit voltage (V_{OC}) of 763 mV-841 mV. DFT calculation was carried out to understand an unique electron transfer mechanism for the DSSC device which may be responsible for the high V_{OC} . More in [DOI: 10.1021/acs.organomet.8b00104](https://doi.org/10.1021/acs.organomet.8b00104) Publication Date (Web): June 19, 2018 (Communication)

