

Designing four naphthalene di-imide based small organic solar cells with 5,6-difluoro-3-oxo-2,3-dihydro-indene non-fullerene acceptors containing melano-nitrile and pyridine carbo-nitrile ring

Usman Ali¹, Ayesha Javed², Hina Ramzan², and Muhammad Shoaib²

¹ICCAS

²University of Agriculture Faisalabad

May 27, 2020

Abstract

Four new molecules namely bis (5,6-difluoro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene) di-malononitrile (NDM-1), 3-fluorothiophen-2-yl) methylene)-5, 6-difluoro-3-oxo-2, 3-dihydro-1H-inden-1-ylidene) acetate (NDM-2), 5, 6-difluoro-3-oxo-2, 3-dihydro-1H-inden-1-ylidene)-3-methyl-2-thioxothiazolidin-4-ylidene) malononitrile (NDM-3) and bis (1-methyl-2, 6-dioxo-1, 2, 5, 6-tetrahydropyridine-3-carbonitrile) (NDM-4) containing central Naphthalene Di-Imide fragment with different end capped acceptors are designed for enhance photovoltaic properties. The absorption strength of designed molecules are between 400 and 490 nm, re-organization energy values vary from 0.0187 eV to 0.0343 eV for electron and 0.0210 eV to 0.0458 eV for hole, open circuit voltages are from 4.39 V to 4.73 V which indicates their better photovoltaic properties as compare to the R (3-methyl-4-oxo-2-thioxothiazolidin-5-ylidene) methyl).

Hosted file

manuscript (1).docx available at <https://authorea.com/users/326676/articles/454718-designing-four-naphthalene-di-imide-based-small-organic-solar-cells-with-5-6-difluoro-3-oxo-2-3-dihydro-indene-non-fullerene-acceptors-containing-melano-nitrile-and-pyridine-carbo-nitrile-ring>