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

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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)-(4,6-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).

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