A theoretical study of substituted indeno[1,2-b]fluorene compounds and their possible applications in solar cells

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This contribution mainly describes the theoretical computations based on density functional theory (DFT), of the anti-aromatic system indeno[1,2-b]fluorene with the aim of understanding the electronic effects of the substituting electron donating and electron withdrawing groups in the 6,12-positions, to investigate their potential role as sensitizers in solar cells devices. Ground state potential energy surfaces were obtained employing the B3LYP/6-31+G(d,p) theoretical level. The low energy electronic transitions were investigated through the TD-DFT method. It was possible to conclude that indeno[1,2-b]fluorine with NH<inf>2</inf>, NO<inf>2</inf>, CN substituents are the best candidates to act as light harvesting and sensitizers in solar cells. © 2015 Elsevier B.V. All rights reserved.