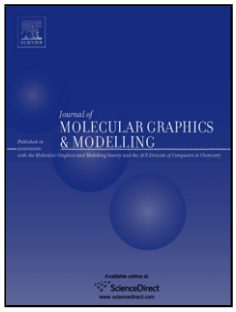

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Monitoring of the Energy levels by heteroatom substitution to hexacene and controlling over singlet fission and Photo-oxidative resistance

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ABSTRACT

The singlet fission is a spin allowed and extremely fast internal conversion process involved in solar cell by which a photo-excited singlet exciton is splitted in to two triplet ones. For effective singlet fission and to increase the efficiency of solar cell, designing of new molecules is an interesting area of research and our current interest. The silicon substituted oligocenes, commonly known as silaoligocenes, are found to be the efficient singlet fission material due their special characteristics. We have shown the SF energy criteria satisfied by the singlet and triplet states of various silahexacene derivatives, and theoretically predicted whether such molecules exhibit fission properties or not. The fluorine atoms have been substituted to various positions of different silahexacenes to manipulate their singlet and triplet energy levels. As fluorine being the most electro-negative substituent, it is capable of lowering frontier molecular orbital energies effectively. Thus, the material can easily match SF energy criteria to compute the SF driving force or triplet-triplet annihilation possibility. The geometries, electronic structures, frontier molecular orbital energies, optimization of excited state and calculation of energies associated with fission process of the substituted hexacene are investigated with well known quantum mechanical methods.

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