

Similarity measures between excited singlet and triplet electron densities in linear acenes: an application to singlet fission

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Resumen

A theoretical framework for modelling the electronic structure of absorbing molecules that may contribute to explain and even predict phenomena where a singlet exciton is converted to triplet is reported. The pathway is suggested to occur when the excited singlet and triplet electron density maps are similarly shaped at Frank Condon states. Calculations were carried for some linear acene excitons from their multielectronic wave functions and corresponding charge maps after a configuration interaction of singly excited determinants. For cases where the singlet fission effect has been reported, charge maps of certain higher energy singlet excitons show a relevant shape similarity with the corresponding lowest triplet. This method could enlighten the way for predicting transit between singlets and triplets of very big systems and also may help to explain experimental phenomena at femto and even attosecond scales.

Palabras clave

Palabras clave de autor: [Singlet-triplet conversion](#); [singlet fission](#); [electron density map](#); [exciton binding](#); [Coulomb-exchange term](#); [acenes](#)

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