

Carbene Based Materials for Organic Solar Cells

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Abstract

Successful strategies for the modelling of singlet fission chromophores – highly efficient organic materials in solar cells, will be demonstrated on a series of theoretically designed NHC-carbene dimers. All compounds are synthetically feasible and thus suitable for practical application. They differ in topology, conformation, and type of substituents, which allows us, using quantum-chemical methods, to reveal the intimate correlation between structure and excited state properties. Several potential candidates for singlet fission chromophores were discovered in the series. The relationship between molecular conformation and singlet fission propensity is demonstrated for the first time.

Keywords: *singlet fission, excited states, photovoltaics, quantum-chemistry*