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Optimization of Ultrafast Singlet Fission in One-Dimensional Rings Towards Unit Efficiency

Singlet fission (SF) is an electronic transition that in the last decade has been under the spotlight for its applications in optoelectronics, from photovoltaics to spintronics. Despite considerable experimental and theoretical advancements, optimizing SF in materials like multichromophoric systems and molecular crystals remains a challenge, due to the complexity of its analysis beyond perturbative methods. Here, we tackle the case of one-dimensional rings, aiming to promote singlet fission and prevent its backreaction. We study ultrafast SF nonperturbatively, by numerically solving a spin-boson model, via exact propagation and tensor network methods. By optimizing over a parameter space relevant to organic molecular materials, we identify two classes of solutions that can take SF efficiency beyond 85% in the nondissipative (coherent) regime, and to 99% when exciton-phonon interactions can be tuned. After discussing the experimental feasibility of the optimized solutions, we conclude by proposing that this approach can be extended to a wider class of optoelectronic optimization problems.

Theme

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