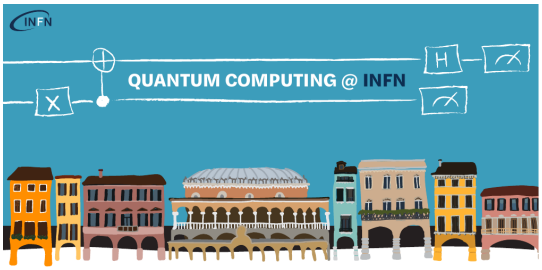

Contribution ID: **21** Type: **not specified**

Optimisation of ultrafast singlet fission in 1D rings towards unit efficiency

Thursday, 31 October 2024 12:20 (20 minutes)

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, optimising SF in extended solids remains a challenge, due to the complexity of its analysis beyond perturbative methods. Here, we tackle the case of 1D rings, aiming to promote singlet fission and prevent its back-reaction. We study ultrafast SF non-perturbatively, by numerically solving a spin-boson model, via exact propagation and tensor network methods. By optimising over a parameter space relevant to organic molecular materials, we identify two classes of solutions that can take SF efficiency beyond 85% in the non-dissipative (coherent) regime, and to 99% when exciton-phonon interactions can be tuned. These results are a promising step towards optimising SF in 2D and 3D extended media. After discussing the experimental feasibility of the optimised solutions, we conclude by proposing that this approach can be extended to a wider class of optoelectronic optimisation problems.

Sessione

Simulazione

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Session Classification: Quantum Simulation