Topic 1: Multi-exciton generation in molecular semiconductors via singlet fission

What to expect

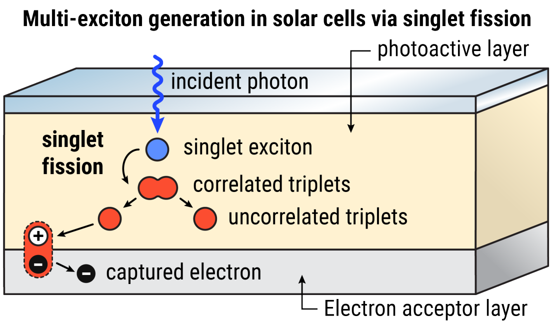
In this project, you will learn about modelling electronic transitions using the theory of open many-body quantum systems. You will familiarize with tensor network methods, open quantum system, and parallel computing on the cluster. Basic knowledge of quantum mechanics and Python is required to approach the tasks.

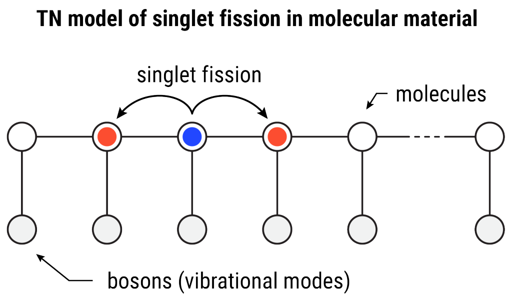
Overview

In organic solar cells (OSCs), incident photons are absorbed by a photoactive material to form excited electronic states, known as *excitons*. Excitons are then transported in the material until they reach an electron acceptor, where they undergo charge separation, producing a photocurrent. However, the short nanosecond lifetime of excitons limits the efficiency of OSCs.

Singlet fission is an electronic processes that is now being explored as a way to improve the efficiency of organic solar cells[1]. In singlet fission, a photo-generated exciton with spin 0 (known as *singlet*) splits into two excitons with spin 1 (known as triplets) in a energy-conserving and spin-conserving transition. This process can improve OSCs efficiency by producing two excitons per absorbed photon, and by increasing the probability for the excitons to reach an electron acceptor, since triplets have a microsecond lifetime.

In this project we will implement a numerical model to study singlet fission in extended solids, which remains a challenge in the field[2]. In particular, we will consider a 1D lattice of molecules and using tensor networks (TNs) to solve a many-body model of singlet fission. After comparing the TNs results with known solutions, we will scale up the model to study how singlet fission scales with the number N of molecules. Finally, we will study the effect of disorder and of the vibrational modes of the molecular lattice.





Tasks

- Implement the singlet fission model for a 1D lattice of molecules using Tree Tensor Networks (TTNs).
- Compare the TTN results with an exact solution (provided in the notes) and study how the TTN results change with the chosen bond dimension.
- Study the effect of local and two-body disorder, to see if it affects the performance of singlet fission. Average over many realisations of disorder by running simulations in parallel on the cluster.
- Introduce the vibrational modes of the molecules, treated as bosons, by embedding one exciton and one boson per site, and study how these affect singlet fission.

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[1] M. J. Y. Tayebjee et al., Journal of Physical Chemistry Letters **6**, 2367 (2015).
[2] K. Miyata et al., Chemical Reviews **119**, 4261 (2019).