Aspuru-Guzik Theoretical Chemistry Group Applications

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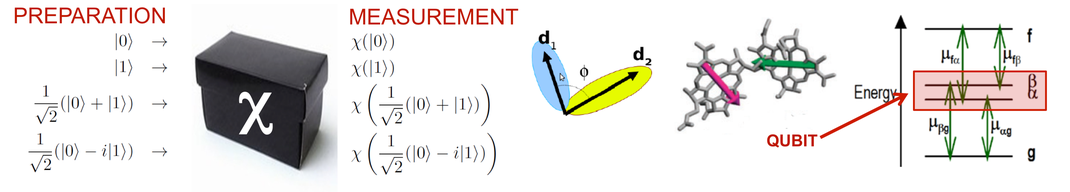
Quantum Process Tomography

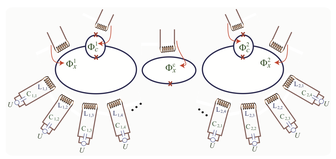
Green sulfur bacteria have a relatively simple photosynthetic structure. Bacteriochloriphylls are assembled in chlorosomes, bodies which have little internal structure. The excitation from the chloroplast is relayed to the transmembrane photosynthetic reaction center through a trimer of the Fenna-Matthew-Olson complex (FMO). FMO serves as an excitonic wire, and has an outstanding efficiency of almost 98%. We are investigating the underlying mechanisms of the energy transport such as quantum coherent hopping and fluctuations in the protein environment.

The *quantum black box* problem (Nielsen, Chuang).



Quantum Simulation of FMO with Superconducting Qubits

Given the importance of FMO, the development and simulations of models for characterizing its behavior has been of great interest. An accurate model must contain many aspects of the physics of the system, including proper characterization of the electron-phonon coupling and environmental decoherence. In an effort to reach more realistic models, we have begun to map the problem onto quantum architectures, where we hope to use the power of quantum simulation on analog quantum systems to lay the foundations for the most accurate and comprehensive calculation to date.

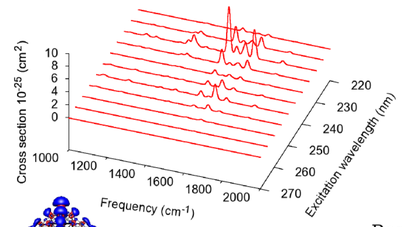


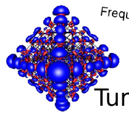
Surface Enhanced Raman Scattering

Raman scattering yields information on the vibrations of a molecule, and hence it helps to characterize and identify them in a non-destructive fashion. However, its intensity is weak. In the late 70's, studies showed that next to a coinage metal particle, the signal is amplified. We are currently elucidating the different enhancement mechanisms and researching which are the important contributions in each case. Our approach includes both theory development, implementation and simulations.

Resonant Raman

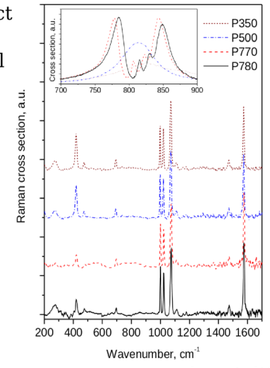
Understanding the Resonant Raman effect is essential in SERS since it metal-molecule interactions contain a manifold of additional electronic levels. We developed a resonant Raman implementation that will enable the study of this effect.





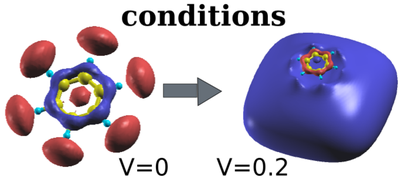
Turbomole

SERS experimental collaborations



Raman spectra measured on 4 different plasmonic substrates (Crozier lab). Inset: Extinction spectra.

Complex boundary conditions



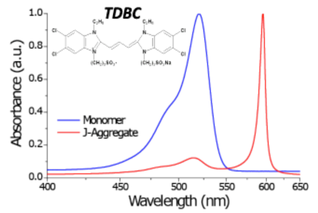
In order to simulate the molecule's complex environment with the nanoparticle, we developed a Poisson-Schrödinger scheme using DFT to obtain a full free energy functional.
The metal is included via its boundary conditions and gate potential.

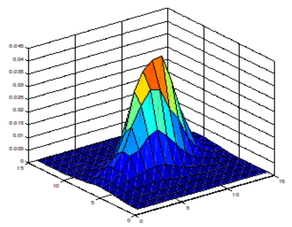
Octopus

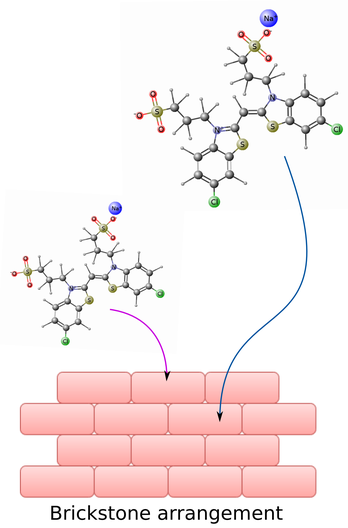
Exciton Dynamics in J-aggregates

J-aggregates are aggregates of cyanine dyes that show an intense and narrow band (the **J-band**) in their absorption spectrum respect to the monomeric species.
They are very efficient light absorbers and are good energy transfer materials because of their high exciton mobility. The exact microscopic mechanism of energy transfer/ exciton motion is still unclear.

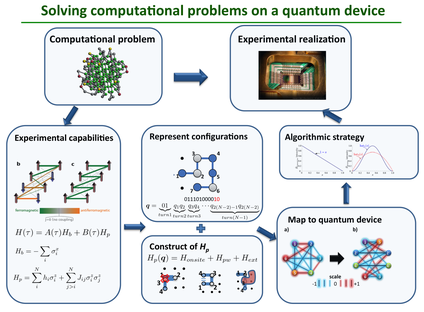
We are working to gain a better understanding of exciton dynamics on 2D films of J-aggregates by using a MCWF (Monte Carlo Wave Function) method. By considering the system as Markovian, we can determine the population at various times for each site as well as information on the self-diffusion.







Protein Folding on a Quantum Computer

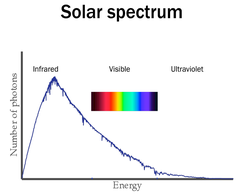


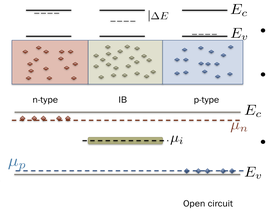
One of the great outstanding challenges of theoretical chemistry is the accurate determination of the folded structures of proteins. The high number of degrees of freedom on a potential surface that is somewhere between quantum and classical makes this problem very difficult.

By mapping a protein to lattice model that is implementable by a current quantum annealing architecture manufactured by DWave, we have accomplished the first protein folding simulation on a quantum device. Quantum annealing promises to be a more effiscient approach for finding the folded configuration when compared to classical search schemes, and as the scalability and power of quantum devices continue to increase, so will the size of proteins we can feasibly fold.

Intermediate Band Photovoltaics

Many researchers are looking for third generation photovoltaic technologies, which are hoped to be more efficient than current systems without increased cost. One such system, the intermediate band (IB) photovoltaic, can ideally absorb more sunlight while still producing large voltages. However, the IB will also cause recombination, decreasing efficiency. Our research has shown that an IB with large bandwidth is necessary to make efficient IB photovoltaics.





- IBPV max efficiency 63%
- Absorb IR and maintain V
- Must minimize recombination