Lab 03 (Simulation2) | Friday 6 October 2017
CHEM 4300-01 | Nanochemistry and Nanotechnology

Resonance Energy Transfer between Nanoparticle and Molecule

Introduction:

Resonant energy transfer (RET) is defined as the transfer of energy from a nanoparticle (that has been irradiated with light) to an acceptor molecule through a dipole-dipole coupling mechanism. Excitation of localized surface plasmon resonance (LSPR) on a metal nanoparticle leads to very strong oscillating dipole moments, and so particles that support LSPR are often good RET donors. Here we will simulate RET from two different types of plasmonic nanoparticle donors: gold@glass nanoshells and gold nanoparticles (see Figure 1 for illustrations), to a dye molecule acceptor (malachite green).

The efficiency of RET between the plasmonic donor and molecular acceptor depends on several factors: the intensity and lifetime of the plasmon, the separation between the plasmonic particle and the molecular acceptor, and the overlap between the scattering spectrum of the plasmonic donor and the absorption spectrum of the molecular acceptor.

In this lab we will simulate RET between a donor nanoparticle and a molecule called *malachite green*. The distance between the donor and the acceptor will range from 2.0-3.0 nm in increments of 0.1 nm.

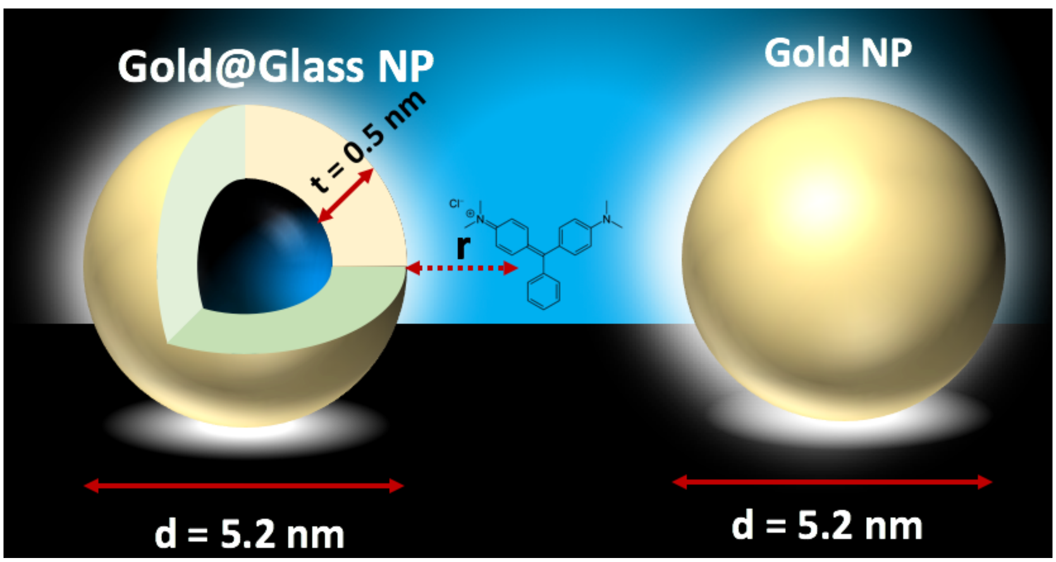

Figure 1 Illustration of Gold@Glass nanoshell and gold nanoparticle. Each particle has a total diameter of 5.2 nm. The Gold@Glass nanoshell consists of a d=4.2 nm glass core with a gold shell of thickness 0.5 nm.

Protocol

We will be using a program called **NanoRET.x** in order to conduct these simulations. Below you will find the instruction on how to run this code.

- Open a new terminal
- Navigate to folder named **NANO_RET**
- Run program **NanoRET.x**
    - Decide which type of nanoparticle you want to use first: Gold or Gold@Glass
    - Name your calculation as follows: ***type of nanoparticle__separation distance***
    - Select the corresponding nanoparticle
    - Enter the separation between the nanoparticle and the molecule
    - Simulation will take approximately 1-2 minutes to run
- Once complete, you will have 3 columns in your terminal. Take note of the values.
- Open the output file in LibreOffice and plot energy transferred vs. separation distance for Nanosphere (Gold) and Nanoshell (Gold TiO_2) for the following distances: 2.0, 2.5, & 3.0)

Post Lab Questions (Note: Chapter 25.12 in Engel in Reid discusses RET; you should consult this along with the primary literature on plasmonics of nanoshells for helpful information in addressing the following questions).

1) Generate plots of energy transfer vs separation distance for both the gold and gold@glass nanoparticles. In the literature, energy transfer vs separation is known to scale as $\frac{1}{r^6}$. Does this scaling seem to fit your data?
2) Plot the scattering spectra for the coupled NP/MG systems and for the lone NP and lone MG systems for the following distances between the donor and acceptor: 2.0, 2.5 & 3.0 for both gold and gold@glass. In which case is the scattering of malachite green most enhanced? Do you notice any unusual features in the scattering spectra of malachite green in any of the cases? If so, describe what you observe. What do you think is causing the spectral features?
3) Which donor (gold or gold@glass) is the most efficient RET donor for malachite green? Explain which properties of the donor are most responsible for its greater efficiency as a RET donor.