Research and Creative Experience for Undergraduates Program (RCEU) Summer 2020

COLLEGE OF SCIENCE
THE UNIVERSITY OF ALABAMA IN HUNTSVILLE

Modeling Decay Dynamics in Systems of Nanoparticles

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This project models the interactions of a layer of quantum dots with metallic nanoparticles thereby simulating a fluorescence lifetime imaging (FLIM) experiment in MATLAB.

Background

Key Abbreviations:

- Quantum dots (QDs): semiconductor colloidal nanocrystals; 5-10 nm spheres of semiconductor molecules such as CdSe
- Metallic nanoparticles (MNPs): spherical metallic nanostructures; 10-100 nm spheres comprised of a single metallic element

QDs are used to develop optoelectronic devices such as lasers, LEDs, and solar panels due to their narrow, bright, and size-dependent emission spectrum, and their broad absorption spectrum as well as other properties.

QDs are influenced by MNPs in two primary ways:

- non-radiative transfer of energy to the MNP through the electric field [described by Förster Resonant Energy Transfer (FRET) or Surface Energy Transfer (SET)]
- increase in radiative decay rate due to the electric field of the MNPs [called plasmonic enhancement]
  - A plasmon is the coherent oscillation of the valence electrons around the MNP with the oscillation of the light exciting it.

Fluorescence lifetime imaging microscopy (FLIM) is an imaging technique that uses the differences in the exponential decay rates of a set of fluorophores (or QDs) to generate an image, as opposed to normal imaging, where variation in fluorescence intensity and/or the variation in the wavelength of light is used to generate an image.

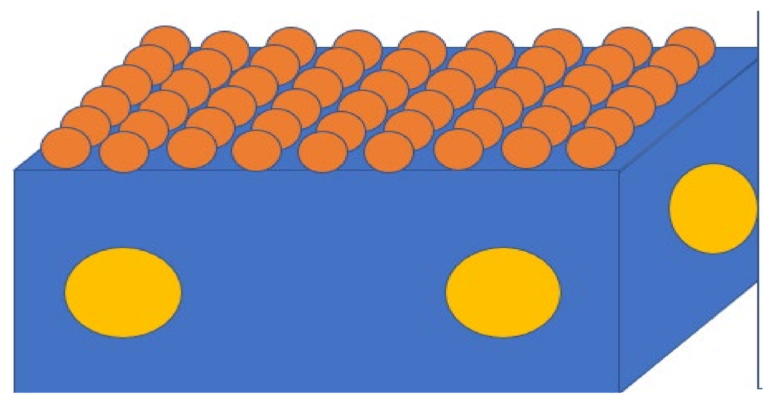

Figure 1
QDs (represented in orange) sitting on a silica layer (represented in blue) with gold MNPs (represented in yellow) embedded in the silica

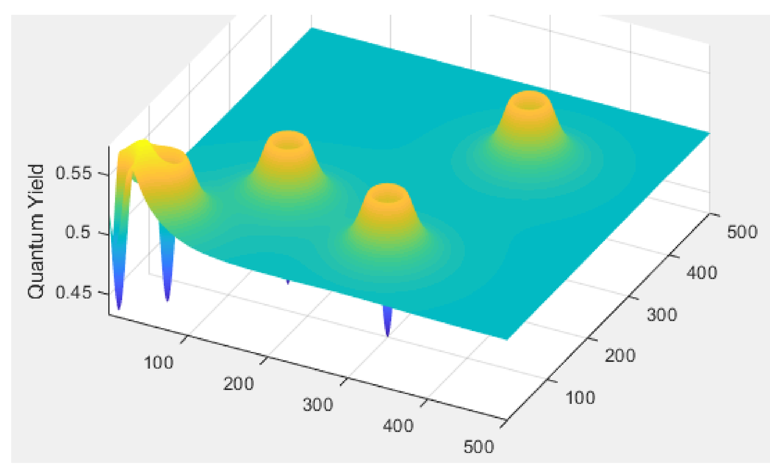

Figure 2
The quantum yield (ratio of emitted per absorbed photons) for all QDs in the array at their locations (x and y axis are distance in the array in nm).

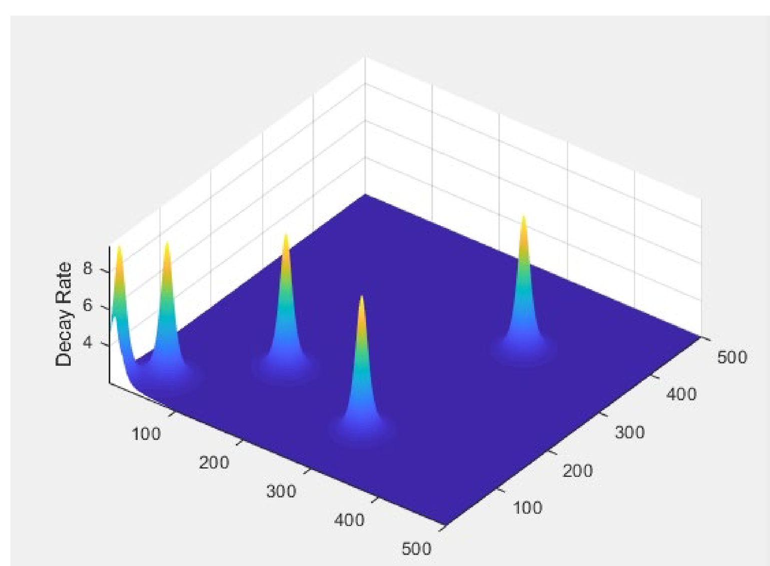

Figure 3
Decay rate: how fast energy in QDs are converted to photons, transfer to MNP, or nonradiatively decay (x and y axis are distance in the array in nm).

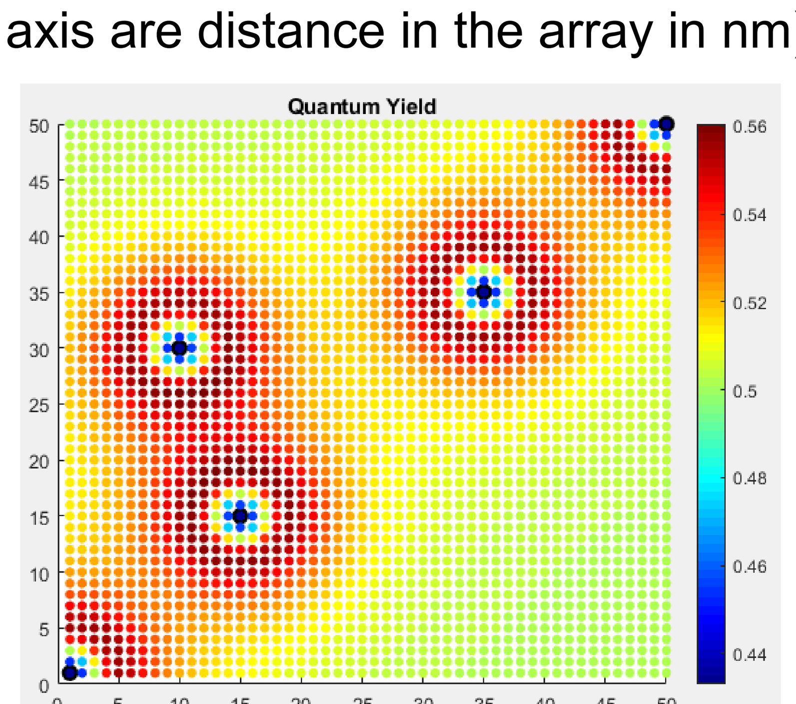

Figure 4
The quantum yield as explained in Figure 3 description is plotted against the position of the QDs as expressed in the x and y axes, where each step represents 5nm.

Method

- MATLAB simulation models interactions between
  - 1 MNP and 1 QD
  - Multiple MNPs and an array of QDs (Figure 2)
- Calculations for this model are based on current research in the interactions between plasmons and excitons (key references below)
- Simulation input parameters include:
  - Spacing of the QDs in the array
  - Center to center distance from MNP to QD directly above
  - Radius of MNP
  - Emission and absorption wavelengths of QDs

Conclusion

The simulation calculates and displays key values for the system consistent with current theory. These can be seen in Figures 3 and 4.

It is an appropriate beginning approximation of a FLIM experiment. There is still much work to be done, such as finding the effect of the presence of MNPs on the transfer of energy between QDs.

Acknowledgements

Thanks to Dr. Seyed Sadeghi for advising this project, and the UAH RCEU Program, the Faculty Senate Finance and Resource Committee, and the National Science Foundation for funding.

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Key References

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