Penn
Materials Science and Engineering
A department of the School of Engineering and Applied Science

Optical Modeling of Self-Assembled Nanocomposites: Structure-Property Relationships

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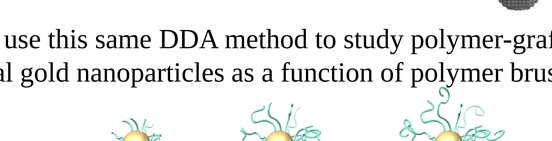
Motivation

- Heating polymer blends of Poly(methyl methacrylate) (PMMA) and Poly(styrene-*ran*-acrylonitrile) (SAN) results in preferential PMMA segregation to the interfaces of the composite[1,2]
- Utilizing this phenomenon, it is possible to make unique and highly controllable morphologies, which have attractive technological applications where controllable nanoparticle (NP) spacing is important: e.g., optical properties ideal for solar cells

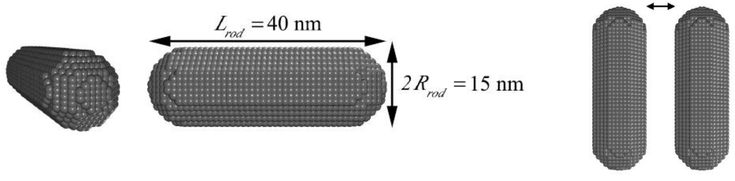


Research Goals

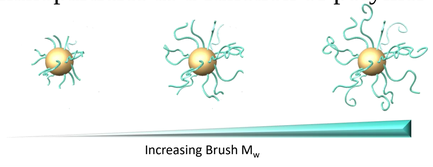
- Study the optical properties of polymer nanocomposites using discrete dipole approximation (DDA) calculations
  - Model discrete polymer-grafted gold NPs with DDSCAT
  - Examine how optical properties of the nanoparticle change when the length of the polymer grafts increases (i.e. spacings)

Identifying Suitable Methodology

- Previously, Hore[3] has shown that DDSCAT simulations can effectively model the optical properties of gold nanorods
  - Utilized DDA method to model gold nanorods as collections of discrete dipoles
  - Examined optical properties as a function of orientation and separations



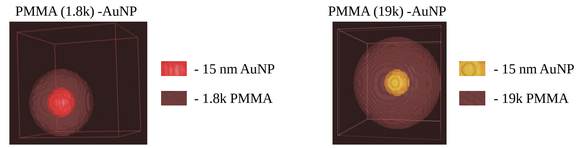
- Can we use this same DDA method to study polymer-grafted spherical gold nanoparticles as a function of polymer brush length?



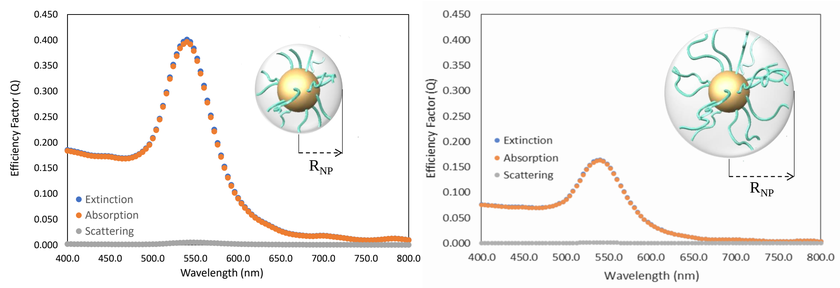
Methods Implemented

- **DDSCAT 7.3**[4,5,6]: Open-source software package that uses discrete dipole approximation (DDA) calculations to model the optical properties of complex targets. This can calculate the light extinction, absorption, and scattering efficiencies across a range of wavelengths
- **nanoDDSCAT**[7]: DDSCAT tool hosted on the nanoHUB website. The "Concentric Ellipsoids" shape format was used to imitate the core-shell structure of the polymer-grafted gold nanoparticles
- **LiteBil**[8]: Visualization tool for DDSCAT shape files, used to generate images of the core-shell structure

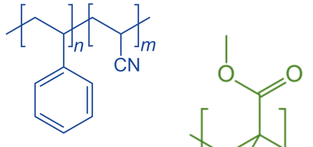
Representative 3D models of PMMA-AuNPs in the same size simulation box

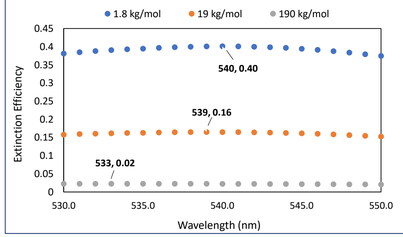


Results



- Both NPs have a 15 nm diameter gold core with PMMA grafts of M_w = 1.8 kg/mol (left) and M_w = 19 kg/mol (right)
- medium: SAN (refractive index n = 1.55)
- graft: PMMA (n = 1.48)





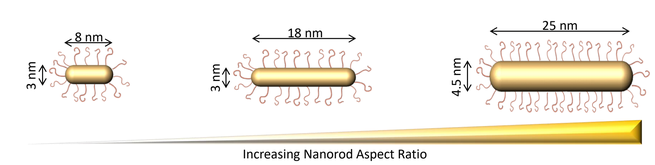
Increasing PMMA length:
- Decrease in peak extinction efficiency
- Slight decrease in corresponding wavelength

Conclusions

- The DDSCAT simulations accurately modeled the optical properties of PMMA-grafted gold nanoparticles
- Additionally, the DDSCAT results were used to examine the effects of the PMMA graft molecular weight on extinction, absorption, and scattering efficiencies

Future Work

- Use DDA simulations to model the optical properties of nanoparticle assemblies as a function of particle dispersion
- Model anisotropic nanoparticles to see the effect of shape on the optical properties of these unique nanocomposite morphologies



- Prepare and characterize nanocomposite films in the lab and compare experimental results with simulation results

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