a. PRF # 58853-UNI6
b. Project Title: Light Initiated Energy Transfer to Petroleum-Derived Molecules Mediated by Hybrid Nanoparticles
c. PI Name and Affiliation: Jonathan J. Foley IV, PhD, William Paterson University

Introduction

This research program aims to advance fundamental understanding of a novel mechanism of light-initiated energy transfer (LIET) between hybrid nanostructures and small organic chromophores. We hypothesize that the unique optical interactions observed in these hybrid nanoparticles can initiate efficient and selective energy transfer to small molecule adsorbates, which has important implications for advancing the ability to refine and transform petroleum-derived feedstocks to desired products.

Results from Year 1

In year 1, the PI and several students successfully addressed one of the principle aims; a quantum dynamical model for the recently-discovered optical phenomenon termed "scattering mediated absorption" (SMA) that occurs in the hybrid metal-dielectric nanostructures illustrated in Figure 1(a); this model was validated against the far-field absorption and scattering properties of such structures as computed by rigorous electrodynamics simulations. A coupling scheme was then developed in order to capture LIET events, specifically resonance energy transfer via dipole-dipole coupling, between the nanostructures and a prototype organic chromophore, malachite green. Through application of this theoretical approach, we predict a 100-fold increase in excitation efficiency by LIET from these nanostructures as compared to the illumination conditions for the lone malachite green system; a proxy of this energy transfer is given by the scattering cross section of lone- and coupled- malachite green in Figure 1(b).

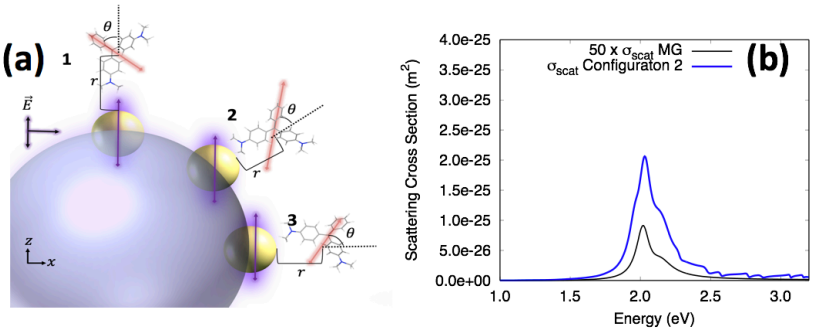

Figure 1 (a) Schematic Illustration of interaction between SMA resonances a HNP and malachite green molecules adsorbed to the surface of the metal sites of the HNP. **(b)** 50-fold enhancement in scattering cross section of malachite green interacting with the HNP through Eq. (1) as compared to isolated malachite green; note spectra of isolated malachite green is scaled by a factor of 50 to aid visual comparison.

Impact on Students and PI

This PRF award has supported several undergraduate and masters students through stipends to conduct research with the PI. These students have been involved in the development and validation of theoretical models, collection and analysis of data, and dissemination of the results. In particular, 2 students were co-authors of a paper describing the results of year 1 that appeared in the Journal of Physical Chemistry C, and one student was supported to travel to a regional and a national meeting of the American Chemical Society to present their findings. The PI's lab has also benefitted from the acquisition of license for a computational electrodynamics package that aided in the development and validation of theoretical models. The PI has benefitted tremendously through this program; financial support during the summer facilitated intensive engagement in this project with several students, and travel support enabled the PI to travel to present results at national and regional meetings. The PI has also leveraged early results to secure funding from the Research Corporation for Scientific Advancement to further efforts in this program of research.