

Optical Spectra of Helical Gold Nanorods: Emergence of the Plasmon Resonance

Harold Hodgins¹, Ian Hamilton¹, Jay Foley², Stephen Gray² ¹Department of Chemistry, Wilfrid Laurier University, Waterloo, Ontario Canada ²Centre for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois USA

Background

 Au_{24} , Au_{40} , and Au_{56} helical gold nanorods have been shown to be energetically stable [1]. Although they have enough electrons to theoretically support plasmon behaviour [2 their length is on the border of being too short[3]. Because they are helical any plasmonic behaviour is likely to be novel



[1] Xiao-Jing Liu, Ian Hamilton, Robert P. Krawczyk and Peter Schwerdtfeger, J. Comp. Chem. 2012, 33, 311-318. [2] A. Eugene DePrince III, Matthew Pelton, Jeffrey R. Guest and Stephen K. Gray, Phys. Rev. Lett. 2011, 107, 196806. [3] GiovanniMaria Piccini, Remco W. A. Havenith, Ria Broer, and Mauro Stener, J. Phys. Chem. C 2013, 117, 17196-17204. [4] Tawada Y, Tsuneda T, Yanagisawa S, Yanai T, Hirao K, J Chem Phys. 2004,120(18):8425-33

Methods

We used TD-DFT as implemented by Gaussian 09 with the lanl2dz [1] basis set and the long range corrected wPBE [5] functional to calculate the Absorbance spectra of the nanorods.





Conclusions / Future Work

A longitudinal plasmon mode appears to be emerging as seen by the red shift in the maximum absorbance peak going from Au_{24} to Au_{56} . Extending the current calculations will help determine if there is a transverse mode at higher energies. Calculating the CD spectra and solving Maxwell's equations for these nanostructures will complement the quantum calculations.





