



UNIVERSITY OF CENTRAL FLORIDA

NANO SCIENCE TECHNOLOGY CENTER
ADVANCED MATERIALS PROCESSING & ANALYSIS CENTER

GRADUATE RESEARCH SEMINAR SERIES

Friday
September 25, 2015

12:15 PM

Research Pavilion
NSTC
Conference Room 475

*Pizza and drinks
will be provided*

Quantum Chemical Studies for the Engineering of Metal Organic Materials

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Metal Organic Materials (MOM) are composed of metal ions as connectors and organic ligands as linkers. Depending on the metal ion and its oxidation state, coordination number, and geometry. MOMs have been found to have high porosity, catalytic, and optical properties. Here we study the gas adsorption, color change, and non-linear optical properties (second harmonic generation (SHG), and two photon absorption (2PA)) of MOMs. These properties can be predicted using theoretical methods, and the results provides experimentalist with tools for rational design and engineering of novel MOMs. Semi-empirical quantum mechanical (SE-QM) calculations were used with the PM7 Hamiltonian (which includes dispersion correction for molecular interactions). Density Functional Theory (DFT) was used to predict the structure and properties in the ground state, and Time Dependent DFT (TD-DFT) was used to consider the evolution of the system and predict the excited states and the optical properties.



In this presentation, the results of multiple projects will be presented. The first topic consist in an effort to aid in the design of gas storage materials. For this goal, theoretical prediction of the molecular absorption capacity of aldoxime coordinated Zn^{+2} based MOMs (previously measured experimentally) was executed with the use of SE-QM methods with PM7 Hamiltonian. The second topic consist in understanding linear absorption properties (color change) of Co^{+2} based complexes after the coordination number is altered. In order to understand the mechanism of the color change TD-DFT methods were employed. The third topic consist of investigation of covalent organic frameworks (COFs) non-linear optical (NLO) properties. DFT calculations were used to predict the hyperpolarizability tensor components with the use of the finite field Berry phase approach. This was done with the purpose of designing an efficient SHG material. The fourth topic consist in theoretical studies to aid on the design and development of in vivo bio-imaging agents for the brain, porphyrin derivatives are theoretically studied using TD-DFT and the mechanism of 2PA enhancement was found.