

Design of Fluophores for Biological Imaging

PROJECT DESCRIPTION

During the internship the student will utilize state-of-the-art computational chemistry tools to explore photophysical processes in molecules. Specific applications could include one-photon and two-photon absorption in fluorescent proteins, resonance Raman spectroscopy to probe initial excited state dynamics, fluorescent nucleobase analogs, and benchmarking of electronic structure methods for challenging structures; recently published papers in these areas are listed below.

References: 1. M. Alaraby Salem and A. Brown, 2015, Two-photon absorption of fluorescent protein chromophores incorporating non-canonical amino acids: TD-DFT screening and classical dynamics, *Phys. Chem. Chem. Phys.* 17, 25563-25571.

2. M.R. Momeni and A. Brown, 2015, Why Do TD-DFT Excitation Energies of BODIPY/Aza-BODIPY Families Largely Deviate from Experiment? Answers from Electron Correlated and Multireference Methods, *J. Chem. Theo. Comp.* 11, 2619-2632.

3. S. Sun and A. Brown, 2015, Simulation of the Resonance Raman Spectra For 5-Halogenated (F, Cl, and Br) Uracils, *J. Phys. Chem. A*, 119 (17), 3961-3971.

4. M. Alaraby Salem and A. Brown, 2014, Two-photon absorption in fluorescent protein chromophores: TDDFT and CC2 results, *J. Chem. Theo. Comp.* 10 (8), 3260–3269.

5. S. Sun and A. Brown, 2014, Simulation of the Resonance Raman Spectrum For Uracil, *J. Phys. Chem. A* 118 9228-9238.

6. M. Gedik and A. Brown, 2013, Computational Study of the Excited State Properties of Modified RNA Nucleobases, *J. Photochem. And Photobiol. A: Chemistry*, 259 25-32.

FACULTY-DEPARTMENT

Science- Chemistry

DESIRED FIELD OF (STUDENT) STUDY

Chemistry; experience with quantum chemistry is preferred

INTERNSHIP LOCATION

University of Alberta Main Campus – Edmonton

Contact: Brendan Cavanagh, Internship Coordinator (Inbound)
University of Alberta International
intern@ualberta.ca

NUMBER OF INTERNSHIP POSITIONS

1

INTERNSHIP START DATE

July 3, 2018

INTERNSHIP END DATE

September 28, 2018

ARE THE DATES FLEXIBLE?

Yes, I am flexible regarding the internship dates. Selected students can contact me to request a date change.