Title: Density-Functional Theory (DFT) Computations on Organic Semiconductors

Program of Study: Chemistry

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Organic semiconductors are an important part of the field of electronics because of properties that place them between insulating and conducting materials. Typically, semiconducting materials are used in electronic components with functions ranging from transistors to LEDs. A determining factor of a material's ability to function as a conductor is the material's band gap which is the energy difference between its ground electronic state and the lowest excited electronic state; a smaller band gap allows for easier electron transfer which promotes conductance. Semiconductors have a band gap intermediate to that of conductors (small band gap) and insulators (large band gap). Organic semiconductors have naturally occurring electronic properties that contribute to their intermediate band gap, as opposed to inorganic materials which rely on manufactured impurities propagating their semiconductive nature. The electronic properties of organic semiconductors are primarily governed by their degree of conjugation, a property which is determined by the delocalization of electrons in p-orbitals and by the geometry of a molecule. Effective conjugation allows for easy movement of electrons throughout the molecule upon excitation and decreases the band gap. This poster will present the determination of electronic properties, such as the band gap, of 3, 4: 3', 4' – bibenzo[b]thiophene (BBT) and several derivatives of this molecule using computational methods, namely Time Dependent Density Functional Theory (TD-DFT) and Equation of Motion Coupled Cluster (EOMCCSD) with different basis sets. Some of these compounds have been reported as useful semiconductors; other, modified, compounds have the potential to increase semiconductivity. Optimal molecular geometries and vibrational frequencies of these compounds will also be computed and presented. Results about the compounds' geometry give insight into their extent of conjugation, and thus allows for evaluating their potential for semiconductivity and also for fluorescence.