Contribution ID: **38** Type: **Poster**

The impact of the solvent media and substituents on the energy band-gap and redox potential of hydroxybenzophenone (HBP) using both experimental and computational methods

The interest of this research is to study the electrochemical properties, energy band-gap and stability of five derivatives of hydroxybenzophenone (HBP). Hydroxybenzophenone derivatives are important compounds that are being used as chromophore in sunshades to protect the human skin from sunburn and are known to be photostable with little to no formation of a photoreactive radical that can penetrate the body to cause DNA damage. HBP are also organic pi–conjugated molecules that can demonstrate a good charge transport and/or electroluminescent properties in their application as organic semiconductors (OSCs).
The aim is to gain insights into the energy band-gap, current peaks and the redox potential of the five derivatives of HBP in different solvent media using both experimental and computational methods. The five derivatives was selected to span the range of those with strong electron withdrawing substituents to those with strongly electron donating substituents. This study will give more insight into their light absorption, photocarrier properties and will also help in their rational design approaches to improve their efficiency as OSCs.
The band gap energy of organic pi-conjugated materials is very important for their application in organic and hybrid electronic devices such as organic light emitting diodes (OLEDs), organic photovoltaic cells (OPVs) and organic field-effect transistors (OFETs). Besides corroborative information that will be gathered from computational approach, it will also helps to gain insight into the preferred type of isomeric form that the derivatives are prone to assume in different solvent media as shown in Scheme 1.

Supported Student

Primary author: ADENIYI, Adebayo (University of the Free State)

Co-author: Prof. CONRADIE, Jeanet (University of the Free State)

Presenter: ADENIYI, Adebayo (University of the Free State)

Session Classification: SIG Poster

Track Classification: SIG Seminar: Chemistry, Material Science and Health Science