World Academy of Science, Engineering and Technology
International Journal of Electronics and Communication Engineering
Vol:15, No:08, 2021

The Effect of Torsional Angle on Reversible Electron Transfer in Donor: Acceptor Frameworks Using Bis(Imino)Pyridines as Proxy

Authors : Ryan Brisbin, Hassan Harb, Justin Debow, Hrant Hratchian, Ryan Baxter

Abstract : Donor-Acceptor (DA) frameworks are crucial parts of any technology requiring charge transport. This type of behavior is ubiquitous across technologies from semi conductors to solar panels. Currently, most DA systems involve metallic components, but progressive research is being pursued to design fully organic DA systems to be used as both organic semi-conductors and light emitting diodes. These systems are currently comprised of conductive polymers and salts. However, little is known about the effect of various physical aspects (size, torsional angle, electron density) have on the act of reversible charge transfer. Herein, the effect of torsional angle on reductive stability in bis(imino)pyridines is analyzed using a combination of single crystal analysis and electro-chemical peak current ratios from cyclic voltammetry. The computed free energies of reduction and electron attachment points were also investigated through density functional theory and natural ionization orbital theory to gain greater understanding of the global effect torsional angles have on electron transfer in bis(imino)pyridines. Findings indicated that torsional angles are a multi-variable parameter affected by both local steric constraints and resonant electronic contributions. Local steric impacted torsional angles demonstrated a negligible effect on electrochemical reversibility, while resonant affected torsional angles were observed to significantly alter the electrochemical reversibility.

Keywords : cyclic voltammetry, bis(imino)pyridines, structure-activity relationship, torsional angles
Conference Title : ICOEM 2021 : International Conference on Organic Electronics and Microdevices
Conference Location : London, United Kingdom
Conference Dates : August 19-20, 2021