THEME: Nanotech for Energy and Environment

TD-DFT theoretical studies of Pyrazoles, Pyrazines and Quinolines for DSSC's

Neredimelli Udaya Sri[1], Mandru V S Prasad[2**] B. Rajani[3]

[1,2]*Molecular Spectroscopy Laboratory, Department of Physics, D.N.R.College, Bhimavaram, W.G.Dt.-534202, INDIA.*

[3]*Govt. College, Kukatpalli, Hyderabad, Telangana.*

**Corresponding author. Mobile: (+91) 9440143723; E-mail: prasad2008mandru@gmail.com

Table of contents

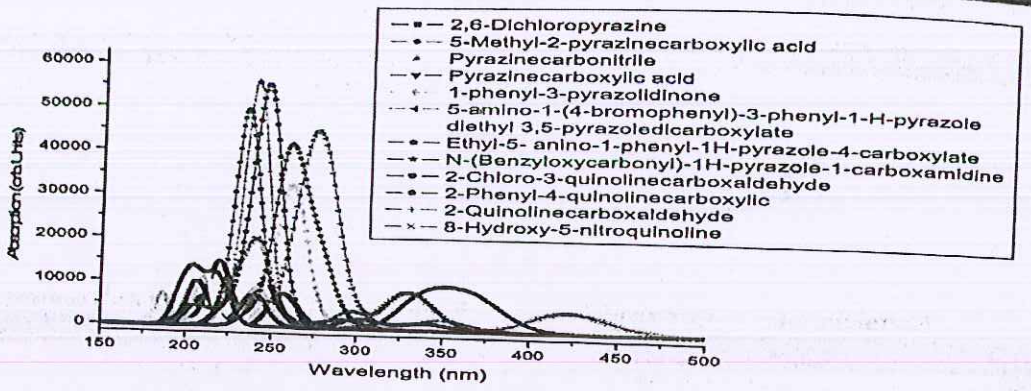

Figure 2. Simulated UV-Visible spectrum of pyrazole, pyrazine and quinoline derivatives derivatives using TD-DFT/6-31G(d) level of theory

ABSTRACT

Pyrazole azo dyes occupy a central place in dye chemistry. Pyrazole dyes are prepared either by coupling of diazopyrazoles with a suitable coupler or by coupling aromatic and heteroaromatic diazonium salts with or aminopyrazoles. Pyrazine (also known as 1,4-diazene) is the heterocyclic compound having two nitrogen atoms in the para position of the six-membered ring, which is very useful for the purpose of NLO applications. The photophysics linear and non-linear optical properties of N-containing heterocycles such as pyrazole, Pyrazine and Quinoline are investigated with density functional theory (DFT) and time-dependent density functional theory (TD-DFT). In this perspective, we present an overview of N-containing heterocycles studied under TD-DFT with a specific focus on its accuracy. To this end, we first summarise recent benchmarks and define an average TD-DFT accuracy in reproducing excitation energies when a conventional approach is used. Next, coupling of TD-DFT with models able to account for different kinds of interactions between a central chromophore and nearby chemical objects is investigated. Examples of application to excitation properties are presented, allowing to briefly describe several recent computational strategies. In addition, an extension of TD-DFT to describe a phenomenon involving interacting chromophores, *e.g.* the electronic energy transfer (EET), is presented to illustrate that this methodology can be applied to processes beyond the vertical excitation. This perspective therefore aims to provide to non-specialists a flavour of recent trends in the field of simulations of excited states in "realistic" situations. Density functional theoretical studies such as geometry optimization, First order hyperpolarizability, HOMO-LUMO energies and quantum chemical calculations have been carried out using B3LYP/6-31G(d,p) basis set.

Keywords: DFT, TDDFT, Heterocycles, HOMO-LUMO, Hyperpolarizability.

(ISBN: 978-81-924726-4-5)

SOUVENIR & ABSTRACTS

2nd International Conference on Nano Science & Engineering Applications -2018

4th to 6th October 2018

Sponsored by TEQIP-III

Organized by

Centre for Nano Science and Technology, Institute of Science and Technology,
Jawaharlal Nehru Technological University Hyderabad (http://jntuhist.ac.in/viewdept/14)
In Collaboration with Center For Advanced Materials (CAM), Qatar University, Qatar.