Tentative Outline

Special Issue for Current Organic Chemistry

Guest Editor(s): Monu Joy and Bijo Mathew

TITLE: Influence of Computational Chemistry on the Mechanistic View of Organic reactions

Aims & Scope:

In recent decades, computational chemistry calculations have been used for various organic chemistry fields such as reaction pathway analysis and spectroscopic assignments due to the theoretical developments and high-speed parallel computers. Understanding the mechanisms of chemical reactions, especially organo-metallic catalysis, bioorganic, heterocyclic and natural product chemistry has been very important and active areas of computational organic chemistry. Computational chemistry is well suited to the mechanistic insights of chemical reactions and it can provide detailed potential energy surfaces (PESs) of various possible reaction pathways followed by the geometrical and electronic properties of reactants, products, intermediates, and transition-state structures, enabling comparisons with various experimental observations such as kinetics, reaction intermediates, isotope effects, and stereochemistry. A systematic insight of various reaction mechanisms and the conception gained from these studies are very useful for further developments and optimization of the reactions and this is, in turn, helps in the design of new reactions and catalysts. Various examples are available in the literature where the advantages and limitations of computational techniques and some challenges in the mechanistic studies followed by the prediction of reactions are also demonstrated/

Keywords: Computational mechanistic study; DFT; Simulation of reaction pathways; Transition state modelling.

Subtopics:

- Quantum chemical approaches to organic reaction mechanism
- Potential energy surface scan and transition state modelling
- Molecular dynamics simulation of reaction pathways
- Computational approaches to organo-metallic based catalysis
- In silico based approaches to the design of new reactions and catalysts
- Challenges in the computational mechanistic studies
- Advantages and limitations of computational techniques in reaction mechanism

Approximate Schedule:

- Manuscript submission deadline: 31 Dec 2017
- Peer review due: 30 Apr 2018
- Revision due: 15 Jun 2018
- Notification of acceptance from the Guest Editor: 30 Jun 2018
- Final manuscripts due: 15 Jul 2018