

MOHD FARID B. ISMAIL**Ph.D. (University of Oklahoma)**

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**EXPERTISE**

Computational Chemistry, Polymers, Organic Synthesis

Dr. Farid's main research interest spans the area of physical and organic chemistry, and includes computational and laboratory work. His main subject of study are organic polymers and polymeric materials including their oligomers and small molecule analogs. Dr. Farid is interested in studying fundamental aspects of the material properties such as the relationship between dielectric constant, viscosity, and diffusion coefficient to the molecular structure of the materials. He utilizes tools such as quantum calculations, molecular dynamics simulations, multi-step organic synthesis, polymer synthesis, and various property measurements to help with his studies.. Currently Dr. Farid's research sponsor is the IPM grant scheme from UPM (formerly known as the Research University Grant Scheme (RUGS)).

CURRENT RESEARCH INTERESTS:

- **The relationship between ionic conductivity and the structure of liquid electrolytes**

Various theories to describe ionic conductivity in liquid electrolytes failed to describe the phenomenon across all types of electrolyte. The reason for the failure is the lack of understanding of the molecular factors controlling the phenomenon. This study aims to determine the structural properties of electrolyte molecules that control ions conduction in the electrolyte molecules. The study employs molecular dynamics simulations and quantum chemical calculations of various organic liquids and oligomers.

- **The extraction of impurities in raw petroleum using ionic liquid**

In this study, model oils tainted with small molecule impurities (sulfur compound, carboxylic acid analogs, metal compounds) are mixed with ionic liquids to determine the effect of various cation and anion types to determine the extraction efficiency. Molecular dynamic simulations are employed to determine the molecular level mechanism/ interaction between the cation and the anion with the impurities.

LINK TO POSTGRADUATE FIELD OF STUDY:

Theoretical and Computational Chemistry, Rubber Chemistry, Polymeric Materials, Molecular Science, Organic Chemistry, Ionic Liquids

ADDITIONAL INFORMATION:

http://profile.upm.edu.my/mohd_farid/profail.html