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Decoding isomer fingerprints using Molecular Spectroscopy: Experiment and theory

Isomers are responsible for biodiversity and bioactivity. Structure dictates properties: An isomer of a potent drug can be toxic. Due to the same composition but different configuration, isomers such as conformers and chiral enantiomers share significant similarities and subtle differences in many properties except for their fingerprint properties. Spectroscopy is a powerful technique to decode fingerprints of isomers when supported by computer powered quantum mechanics. Scientific discoveries in digital age is moving from assisting and analyzing results of spectral characterization to guided designing, controlling and driving experiments with more rational knowledge. Physical properties of almost all materials should be predictable, in principle, by solving the quantum-mechanical equations governing their constituent electrons. This presentation will cover a broach spectrum of theory driven discoveries in molecular spectroscopy at Swinburne University through international collaborations in recent years. In particular, the narrative of collaboration leading to breakthrough of the structure of organometallic compound ferrocene using IR spectroscopy will be presented. I will also report our recent studies using electron momentum spectroscopy (EMS), X-ray photoemission spectroscopy (XPS), nuclear magnetic resonance (NMR) spectroscopy and UV-Vis spectroscopy to decode the fingerprints of isomers and their intramolecular hydrogen bonding interactions of isomers with biological and pharmaceutical applications. Ferrocene, anticancer drugs, amino acids and other organic compounds such as furfural and tetrahydrofuran etc will be discussed.

Speaker Biography

Feng Wang (PhD Theoretical/Computational Chemistry, Spectroscopy) is Professor of Chemistry and Deputy Chair of Department of Chemistry and Biotechnology at Swinburne University of Technology, Australia. She received her PhD degree at the University of Newcastle (Australia, 1994), worked at the University of Waterloo (1994-1996) as an NSERC Canada International Postdoctoral Fellow and Research Fellow at School of Chemistry, The University of Melbourne (1996-2000). After a short period at a supercomputer centre, she joined Swinburne University of Technology in 2003. She has led many theoretical/computational chemistry driven discoveries in a broad spectrum of applications in medicinal, biological, solar energy etc in chemistry and physics and has published over 150 peer reviewed journal articles. She is Honorary Professor at School of Chemistry, University of Melbourne, Fellow of RACI and Fellow of the AIP. She also serves on national scientific research committees such as the National Computational Merit Allocation Committee (NCMAC, Australia) and has been an expert panel member for National Research Councils including Ireland, Czech Republic, Portugal, Romania and Canada (Quebec) etc.

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