学 术 报 告

题　目：Computational Chemistry Led Molecular Discoveries At Swinburne University (Australia)

报告人：Professor Feng Wang，Swinburne University of Technology

时　间：2016年06月23日（周四）上午10：00

地　点：中科院固体所大楼221会议室

报告摘要：

Computational (click) chemistry has become a more and more important technique in scientific discovery process. It has been recognized that the computational chemistry methods "can be used to study all kinds of chemistry; from the molecules of life to industrial chemical processes. Scientists can optimise solar cells, catalysts in motor vehicles or even drugs, to take but a few examples."(http://www.nobelprize.org/nobel_prizes/chemistry/).

In this presentation, computational chemistry led molecular discoveries at Swinburne University of Technology (Australia) in recent years will be showcased in a number of fronts through international collaborations. It will cover a broad spectrum of close collaboration in physical chemistry and chemical physics between computational chemistry/molecular modeling and experimental (spectroscopic) measurements, leading to new discoveries. The presentation will cover a recent study of gamma-ray spectroscopy of positron-electron annihilation of alkanes, the applications of spectroscopy in areas such as new organic dye sensitized solar cells (DSSCs). The narrative of recent collaboration with Univ. Melbourne (physics and chemistry) and Australian Synchrotron of ferrocene (catalysis) study using high resolution IR spectroscopy in the past four years will be presented.

报告人简介：

Feng Wang （王凤）obtained her PhD degree in Theoretical/Computational Chemistry from University of Newcastle (Australia) in 1994, after her BSc (Physical Chemistry, 1983) and MSc (Quantum Chemistry by Research,1986) degrees, both from Sichuan University (China). Dr Wang took up the prestigious Natural Science and Engineering Research Council (NSERC) Canada International Postdoctoral Fellowship Award at Department of Chemistry, University of Waterloo during 1994-1996. She returned Australia in 1996 to take up a Research Fellow position at School of Chemistry, The University of Melbourne until 2001. After a brief period in VPAC as a Computational Scientist (2001-2002), Dr Wang joined Swinburne University of Technology as a Senior Lecturer (2003) in Computational Science, and was promoted to Associate Professor (2005) and Professor (2009). She is Professor of Chemistry since 2011. Professor Wang has been a leading researcher in physical chemistry, computational chemistry, molecular spectroscopy and molecular physics. Her expertise in molecular simulation/modelling and quantum chemistry enables her to expand to broader areas of biotechnology, nanotechnology and materials sciences, bridging state-of-the-art supercomputing with synchrotron sourced spectroscopy.

Professor Wang is elected Fellow of Royal Australian Chemical Institute (RACI C CHEM) and elected Fellow of Australian Institute of Physics (AIP). She teaches undergraduate students of all levels, supervises research projects for honours students and PhD students. She has been PhD supervisor since 2003. Professor Wang has published nearly 150 refereed career articles in high impact international journals and has been a leading researcher in Physical Chemistry.

For more information: http://www.swinburne.edu.au/science-engineering-technology/staff/profile/index.php?id=fwang

https://www.researchgate.net/profile/Feng_Wang76