# 量子材料科学中心
# International Center for Quantum Materials

Seminar

# Structure and Dynamics of Water-Solid Interfaces

**Dr. Angelos Michaelides**
**University College London**

**Time: 4:00 pm, Mar. 30. 2012 (Friday)**
**时间：2012年3月30日 （周五）下午4:00**
**Venue: Conference Room A (607), No. 5 Science Building**
**地点：理科五号楼607会议室**

## Abstract

Some of our work in which surprisingly strong quantum nuclear effects are predicted in adsorbed water overlayers will be discussed. I will show how zero point motion and quantum tunneling can lead to hydrogen bond symmetrisation in certain ice overlayers on metal surfaces (PRL 104, 066102 (2010)) and structures resembling the superionic ice X phase of water are predicted. Also the very general role of quantum nuclear effects in altering hydrogen bond lengths and strengths will be discussed (PNAS 106, 6369 (2011)). Time permitting our recent work on the development of improved van der Waals functionals for DFT (JPCM 22, 022201 (2010); PRB 83, 195131(2011)) will be discussed as well as our recent suggestion that the surface of crystalline ice behaves like an amorphous material (Nature Mater 10, 794 (2011)).

## About the Speaker

Angelos Michaelides obtained a PhD in Theoretical Chemistry in 2000 from The Queen's University of Belfast. Following this he worked as a post-doctoral research associate and junior research fellow at the University of Cambridge and then at the Fritz Haber Institute, Berlin, as an Alexander von Humboldt research fellow. Subsequently he was promoted to staff scientist and research group leader at the Fritz Haber Institute. In 2006 he moved to University College London, where since 2009 he has been Professor of Theoretical Chemistry.

He has received a number of honours and awards for his research including the Royal Irish Academy Young Irish Chemist of the Year (2000), a visiting professorship at École Normale Supérieure de Lyon (2004), and a European Young Investigator Award (2005). He was also the 2010 recipient of the Royal Society of Chemistry Marlow Award "For his innovative contributions in broad areas of surface and physical chemistry, with particular relevance to heterogeneous catalysis and improved understanding of the water-ice interface". He currently holds a European Research Council Start-up Grant, is an Academic Editor for AIP Advances, and since 2011 has been Director of the Thomas Young Centre: The London Centre for the Theory and Simulation of Materials

His current research focuses on the application and development of computer simulation techniques to study catalytic and environmental interfaces, with water being a major focus.