



Seminar

Cold water and ice: Insights from computer simulations

Angelos Michaelides

Thomas Young Centre, UCL, London, UK



Time: 4:00Pm, Nov. 22, 2018 (Thursday)

时间: 2018年11月22日 (周四) 下午4:00

Venue: Room W563, Physics building, Peking University

地点: 北京大学物理楼, 西563会议室

Abstract

Recent work from our research group in which we are trying to understand the intimate molecular level details of water freezing will be discussed. A particular emphasis will be placed on the role the surfaces of foreign materials play in accelerating the nucleation process [1-4] and on the dynamical nature of the nucleation event.

1. M. Fitzner, G. C. Sosso, S. J. Cox and A. Michaelides, *J. Am. Chem. Soc.* 137, 13658 (2015)
2. G. Sosso et al., *J. Phys. Chem. Lett.* 7, 2350 (2015)
3. A. Kiselev et al, *Science* 355, 367 (2017)
4. M. Fitzner et al., *Nature Comm.* 8, 2257 (2017)

About the speaker

Angelos Michaelides obtained a PhD in 2000 from The Queen's University of Belfast. Following this he did post-docs in Cambridge and Berlin. In 2006 he moved to University College London, where since 2009 he has been a full Professor.

Research in his group aims at understanding important phenomena in surface- materials- and nano-science. Using concepts from quantum mechanics and statistical mechanics, his team applies and develops methods and computer simulations to study processes of relevance to catalysis - such as the properties of metal surfaces and chemical reactions at surfaces - and processes of environmental relevance - such as the nucleation of ice or the dissolution of salts. Water and ice are major focuses of their work. For more information see www.chem.ucl.ac.uk/ice

Michaelides has received a number of honours and awards including the Marlow Award and Corday-Morgan Prize from the Royal Society of Chemistry. Since 2011 has been a Director of the Thomas Young Centre: The London Centre for the Theory and Simulation of Materials and since 2013 he has been an Associate Editor of the *Journal of Chemical Physics*.