

中心系列讲座 ICQM Weekly Seminar Series

A Molecular Perspective of Water at Metal Interfaces



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Time: 4:00 pm, Jun. 12, 2012 (Tuesday) 时间: 2012年6月12日 (周二)下午4:00 Venue: Room 607, Conference Room A, Science Building 5 地点: 理科五号楼607会议室

Abstract

Water-solid interfaces are ubiquitous and of the utmost importance to industry, technology and many aspects of daily life. Despite countless studies from different areas of science, detailed molecular-level understanding of water-solid interfaces comes mainly from well-defined studies on flat metal surfaces. These studies have recently shown that a remarkably rich variety of structures form at the interface between water and seemingly simple flat metal surfaces. Here we discuss a brief selection of some of the most exciting examples of recent work in this area and the underlying physical insight and general concepts that emerge about how water binds to surfaces. Moreover, special attention will be paid to the role of van der Waals (vdW) in the water-metal interaction by means of recent, improved vdW density functionals. A brief perspective on the outstanding problems, challenges, and open questions in the field will also be provided.

About the Speaker

Dr. Javier Carrasco got his Ph.D from the University of Barcelona in 2006. Then, he worked with a Humboldt Fellowship in the Fritz-Haber Institute of the Max-Planck Society and a Newton Fellowship in the University College London, consecutively from 2007 to 2011. Since 2011 he moved to Madrid for a permanent position as a Raman y Cajal Research Fellow in the Institute of Catalysis and Petroleochemistry of the Spanish national Research Council. His main focus is on a molecular level understanding of water-solid interfaces using ab-initio theoretical methods.