



Chinese Academy of Sciences  
**Key Lab for Biomedical Effects of  
Nanomaterials and Nanosafety**

中科院纳米生物效应与安全性重点实验室



## 学术报告通知

**CAS NS Forum (NO. 282)**



**演讲者: De-en Jiang**

**Associate Professor with Tenure**

**美国加州大学Riverside分校, 化学系**

**题目: In Silico Materials Chemistry**

**时间: 2017年6月27日 (周二) 上午9:00 -11:00**

**地点: 中科院高能物理研究所, 主楼419会议室**

**主持人: 赵丽娜 副研究员**

### 报告摘要:

Function is key to development of new materials and chemistry. To design a material for a specific function, one needs to account for interaction, energetics, and dynamics to simulate the process. Modern computational software and hardware now allow us to design materials, predict structures, and simulate function for some well-defined systems, indicating the great potential of materials design for complex systems in the near future. In this talk, I will discuss our recent efforts in understanding the atomically precise, ligand-protected metal nanoclusters; simulating ion-gated porous graphene membranes for gas separation; controlling the surfaces and interfaces for catalysis. In each of the studies, one will see a close interplay between computation and experiment, demonstrating that computation or an experiment *in silico* is now a valuable tool to drive advances in materials chemistry.

### 个人简介:

#### Career Highlights

- Presidential Early Career Awards for Scientists and Engineers
- 196 peer-reviewed publications: JACS (15), Angew. Chem. (6), Nano Lett. (4), ACS Nano (3), Nature Comm. (2)
- H-index 54; 8823 total citations (from Google Scholar; accessed 9 June 2017)
- Chair and organizers for 17 meeting and symposia on materials and energy
- Lead editor of a Wiley book (488 pages): "Graphene Chemistry: Theoretical Perspectives"
- 138 invited conference talks and seminars

#### Education

- Peking University, Beijing, China, B.S., 1997, Chemistry
- Peking University, Beijing, China, M.S., 2000, Physical Chemistry
- o Advisor: Prof. Youchang Xie (now emeritus)
- University of California, Los Angeles, Ph.D., 2005, Physical Chemistry
- o Advisor: Prof. Emily Carter (now at Princeton University)
- Oak Ridge National Laboratory, Oak Ridge, Postdoctoral, 2006
- o Advisors: Dr. Sheng Dai and Dr. Bobby Sumpter