

CSRC Short Course on Molecular Materials and Device Computation

16-20 July, 2018

Program

	Mon, 16/7	Tues, 17/7	Wed, 18/7	Thur, 19/7	Fri, 20/7
8:30 -	Registration				
9:00 – 10:15	Materials Informatics (郭鸿) Molecular Electronics (郭雪峰)	MOMAP 有机材料设计平台的理论基础 I (牛英利)	经典和量子随机热力学基础 (全海涛)	量子跳跃轨迹的热和功 I (柳飞)	Quantum fluctuation theorems and Information thermodynamics I (Sagawa)
10:15 – 10:45	tea break, discussions				
10:45 – 12:00	Overview of molecular device computation (帅志刚)	MOMAP 有机材料设计平台的理论基础 II (牛英利)	双热库 Feynman 棘轮: 设计与实验 (全海涛)	量子跳跃轨迹的热和功 II (柳飞)	Quantum fluctuation theorems and Information thermodynamics II (Sagawa)
12:00 – 14:00	lunch break				
14:00 – 15:15	DFT 理论基础 (季威)	材料虚拟筛选: 从描述符到机器学习 (覃一发)	量子输运 Nanodcal 软件和求解 KS-DFT 方程的 RESCU 软件 (阮璐风)	光采集分子激发态迁移的量子动力学 I (吴建澜)	
15:15 – 15:45	tea break, discussions				
15:45 – 17:00	非平衡格林函数理论 (邢燕霞)	MOMAP 有机材料设计平台操作和案例 (闫丽慧)	Nanodcal 软件和 RESCU 软件计算案例 (阮璐风)	光采集分子激发态迁移的量子动力学 II (吴建澜)	

参考文献和网站 (其他阅读材料和课件会陆续在暑期班网页发布)

- [1] <http://www.momap.net.cn/>
- [2] <http://hzwtech.com/channel.jsp?id=11>
- [3] Christopher Jarzynski, *Annu. Rev. Condens. Matter Phys.* **2**: 329-351 (2011)
- [4] J Bang, R Pan, TM Hoang, J Ahn, C Jarzynski, HT Quan, T Li, arXiv:1711.04968
- [5] F Liu, *Progress in Physics* **38**: 1-62 (2018) (arXiv:1710.02311)
- [6] Ken Funo, Masahito Ueda, Takahiro Sagawa, arXiv:1803.04778
- [7] Takahiro Sagawa, arXiv:1712.06858