

# 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
<b>8:30 -</b>	Registration				
<b>9:00 – 10:15</b>	Materials Informatics (郭鸿)	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)
<b>10:15 – 10:45</b>	tea break, discussions				
<b>10:45 – 12:00</b>	Overview of molecular devices (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)
<b>12:00 – 14:00</b>	lunch break				
<b>14:00 – 15:15</b>	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)	
<b>15:15 – 15:45</b>	tea break, discussions				
<b>15:45 – 17:00</b>	非平衡格林函数理论 (邢艳霞)	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)	

\*to be confirmed

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