

中国科学院  
国科大



## UNDERSTANDING MOLECULAR SIMULATION

CECAM / KITS / IoP SUMMER SCHOOL

Beijing, July 29 – August 5 2018

Organizers:

**Daan Frenkel**, University of Cambridge, UK  
**Ignacio Pagonabarraga Mora**, CECAM, Switzerland  
**James Farrell**, IoP CAS, Beijing  
**Jure Dobnikar**, IoP CAS, Beijing

Contact and school secretary:

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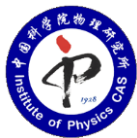
This is a week-long school that offers a program focusing on numerical techniques for the study of properties of many-particle systems. It targets PhD and postdoctoral researchers who want to learn these techniques to study topics in physics, chemistry or biology. The course may also be followed by advanced MSc students. It offers a recap of the statistical mechanics relevant for molecular simulation and addresses basic and advanced simulation techniques including Monte Carlo, molecular dynamics, free energy calculations, rare events and coarse graining without discussing particular software packages.

The school consists of an integrated program of lectures and hands-on exercises. The book "Understanding Molecular Simulation" by Frenkel and Smit will provide the basis of the lectures. This will be supplemented by exercise handouts and copies of the lecture slides. A poster session will provide the participants an opportunity to present their research in an informal setting.

There will be two special additional topics, one on machine learning and its applications in condensed matter and biological physics and the second one on mesoscopic modelling of the fluid flow.

The school starts on Sunday, July 29<sup>th</sup> at 16:00 in the afternoon and ends on Sunday, August 5<sup>th</sup> in the morning. The days are roughly divided as follows:

- **AM: Lecture** (9:00 – 10:30) / **Break** / **Lecture** (11:00 – 12:30)
- **Lunch break** (12:30 – 14:30)
- **PM: Lecture** or **Exercises** (14:30 – 16:00) / **Break** / **Exercises** (16:30 – 18:30)
- **Dinner**



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## TENTATIVE DAY-BY-DAY SCHEDULE

DATE		ACTIVITY	LECTURER
Sunday July 29 <sup>th</sup>	AM	<b>ARRIVAL / REGISTRATION</b>	James Farrell ( <b>IoP</b> )
	PM	<b>Python &amp; Programming Basics</b>	
Monday July 30 <sup>th</sup>	AM	<b>Introduction to Statistical Thermodynamics;</b> <b>Basic Simulation Techniques &amp; Ensembles</b> <b>Monte Carlo</b> , Parallel Tempering	Daan Frenkel ( <b>U. Cambridge</b> )
	PM	<b>Molecular Dynamics</b> Exercise Class	
Tuesday July 31 <sup>st</sup>	AM	<b>Linear response theory</b> , diffusion... <b>Computing observables</b> : pressure, radial distribution function <b>Other ensembles</b>	Daan Frenkel ( <b>U. Cambridge</b> )
	PM	Exercise Classes	
Wednesday August 1 <sup>st</sup>	AM	<b>Free energy calculations</b> : Thermodynamic integration, Umbrella sampling, acceptance ratio, Widom insertion <b>Phase coexistence</b>	Daan Frenkel ( <b>U. Cambridge</b> )
	PM	Exercise Classes	
Thursday August 2 <sup>nd</sup>	AM	<b>Advanced MD</b> : Constraints, Rare events	Erik Lijten ( <b>Northwestern U.</b> )
	PM	<b>Modelling long range interactions</b> : Electrostatics Exercise Classes	
Friday August 3 <sup>rd</sup>	AM	<b>Mesosopic modelling of fluid flow</b> Dissipative Particle Dynamics, Multi Particle Collision Dynamics	Ignacio Pagonabarraga ( <b>CECAM</b> )
	PM	Lattice Boltzmann Exercise Classes	Mincheng Yang ( <b>IoP</b> )
Saturday August 4 <sup>th</sup>		<b>Machine learning</b> Exercise class: big data set, extract correlations; train simple neuron net	Alpha Lee ( <b>U. Cambridge</b> )
Sunday August 5 <sup>th</sup>		<b>SOCIAL PROGRAM / DEPARTURE</b>	