

**Preliminary Program for the Third NBIA Meeting on ESS Science, June 24-28, 2013**

*Only 20 students will take part on the hand on exercises. "ESS Science: Opportunities & Ideas" session is intended to give the participants an opportunity to discuss on what they think is most important to develop a good neutron facility, including instrumentation, sample preparation laboratories, software, hardware, etc..*

<i>Day/Time</i>	<i>Lecturer</i>	<i>Topic</i>
<i>Monday, 1<sup>st</sup> day</i>		
8:00 am - 9:15 am	<b>Registration &amp; Welcome</b>	
9:15 am - 10:30 am	Teresa Head-Gordon (UC, Berkeley)	Computing Experimental Observables from Molecular Simulation: Insights and Predictions
10:30 am - 11:00 am	Coffee break	
11:00 am - 11:45 pm	Tobias Unruh (Erlangen University)	Combination of QENS and MD simulation for soft matter research
11:45 am - 12:15 pm	Janez Mavri (National Institute of Chemistry)	Classical Molecular Dynamics Simulations of Hydrated Proteins
12:30 pm - 2:00 pm	Lunch	
2:00 pm - 2:30 pm	Andrew Jackson (ESS)	Nanoscale Structural Analysis with Neutrons
2:30pm - 3:00 pm	Mark Telling (ISIS)	Quasi-Elastic Neutron Scattering: A Tool for the Study of Molecular Dynamics
3:00 pm - 3:30 pm	<i>Posters</i> Coffee Break	
3:30 pm - 5:15 pm	Andrew Jackson (ESS)	<b>SANS Tutorial</b> - Students chose project, hands on exercises
<i>Tuesday, 2<sup>nd</sup> day</i>		
9:00 am - 9:45 am	Roger Pynn (Indiana University)	A Practical Guide to doing a SANS Experiment at a National Neutron Facility
9:45 am - 10:30 am	Dimitri Argyriou (ESS)	ESS Science: Opportunities & Ideas
10:30 am - 11:00 am	Coffee break	
11:00 am - 11:45 am	Lise Arleth (NBI-KU)	Combining SAXS and SANS to investigate biomolecular systems
11:45 am - 12:15 pm	Jörg Pieper (University of Tartu)	QENS and Optical Spectroscopy in Photosynthesis Research
12:30 pm - 2:00 pm	Lunch	
2:00 pm - 3:45 pm	Mark Telling (ISIS)	<b>QENS Tutorial</b> - Students chose project, hands on: Data analysis etc
2:00 pm - 3:45 pm	ESS Scientists	Round Table with ESS Scientists
4:00 pm - 5:00 pm	Students clip presentations: 3 minutes clip to show their research work	
5:00 pm - 6:30 pm	Beer party and posters	

<i>Wednesday, 3<sup>rd</sup> day</i>		
9:00 am - 10:30 am	<b>2 Students: Working groups</b>	
10:30 am - 11:00 am	Coffee Break	
11:00 am - 11:45 am	Dmitri Svergun (EMBL)	Computational methods for the analysis and interpretation of small-angle scattering data
11:45 am - 12:15 pm	Ritva Serimaa (University of Helsinki)	X-ray and neutron scattering studies on natural polymer based materials
12:30 pm - 2:00 pm	Lunch	
2:00 pm -	Excursion & Conference dinner Viking Museum in Roskilde sponsored by the ESS	
<i>Thursday, 4<sup>th</sup> day</i>		
9:00 am - 9:45 am	Neal Skipper (UCL)	SANS and QENS studies of layered clay and graphite materials
9:45 am - 10:30 am	Juergen Eckert (USF)	What are small molecules doing inside large pores?
10:30 am - 11:00 am	Coffee break	
11:00 am - 11:30 pm	Jacob Judas Kain Kirkensgaard (NBI-KU)	Combining SANS and computational modeling for structural determination in star polyphile liquid crystals
11:30 am - 12:00 pm	Margarita Krutyeva (JCNS)	Dynamics of macromolecules - NMR & neutron scattering
12:15 pm - 1:30 pm	Lunch	
1:30 pm - 4:00 pm	<b>2 Students: Working groups</b>	
1:30 pm - 4:00 pm	Guided Tour for the senior scientists: Natural History Museum of Denmark <a href="http://geologi.snm.ku.dk/english/udstillinger/flora_danica/">http://geologi.snm.ku.dk/english/udstillinger/flora_danica/</a>	
4:00 pm - 4:30 pm	Students coffee break	
4:30 pm - 6:00 pm	<b>2 Groups of Students (30 minutes each group)</b>	Student presentations on their results
<i>Friday, last day</i>		
9:00 am - 9:45 am	Sandrine Lyonnard (DSM/INAC-CEA)	Looking into fuel cell electrolytes with QENS & SANS
9:45 am - 10:30 am	Dorthe Posselt (RUC)	Structure and dynamics of phospholipid membranes doped with 1-alkanols
10:30 am - 11:00 am	Coffee break	
11:00 am - 11:45 pm	Emiliano Fratini (University of Florence)	Structure and dynamics in concentrated protein solutions
11:45 am - 12:30 pm	Heloisia N. Bordallo (NBI-KU)	Biomaterials, Complexity and Neutrons
12:30 pm - 2:00 pm	<b>Lunch and Good Bye</b>	