HPC@FKF Symposium 2018

Thursday 18. January 2018 – 09:00-20:00

Venue: Hotel Plaza

08:30-09.00 Arrival, breakfast available

09:00-09:15 Welcome (Hans Jørgen Aagaard Jensen)

09:15-10:30 Session I
Chairman: Ilia Solov'yov

Jógvan Magnus Haugaard Olsen	Modeling response properties of large molecular systems
Dalibor Hršak	Polarizable density embedding in coupled cluster
Weria Pezeshkian	Membrane properties at large length scales
Vikas Dubey	Mechanism of proton redistribution in the Gastric Proton Pump
Claus Nielsen	Spin dynamics and the radical pair mechanism

10:30-11:00 Coffee/tea break

11:00-12:00 Session II
Chairman: Himanshu Khandelia

Ida Friis	Cryptochrome interactions
Nicky Mattsson	Coarse-Graining via the Mori-Zwanzig formalism
Erik Kjellgren	State specific and linear response approaches to excitation energies
Peter Reinholdt	Development of Force Fields for Polarizable Embedding

12:00-13:15 Lunch

13:15-14:15 Session III

Chairman: Carsten Svaneborg

Igor Gula	MD simulations to study the elastic properties of polymer materials and to investigate damage and wear mechanisms
Vasili Korol	Introduction to VIKING
Julie Stendevad	Optical Properties of C5-substituted Pyrimidine Nucleosides
Angela Barragan	TBA

14:15-15:00 Coffee/tea and cake

15:00-16:30 Session IV

Chairman: Jógvan Magnus Haugaard Olsen

Ilia Solov'yov	Quantum biology and computational physics
Jacob Kongsted	Is Quantum Chemistry relevant for the Biological Sciences?
Michael Pedersen	Serpins, nucleic acids and bacteria
Himanshu Khandelia	Computational membrane biophysics
Carsten Svaneborg	Modelling of polymer materials
Hans Jørgen Aa. Jensen	Method development in the Dalton and Dirac programs

16:30-18:00

Beer/Soft drinks and informal discussions ...

18:00-20:00 Dinner