

ESI/CECAM Workshop on  
“Physics and Chemistry at Fluid/Fluid Interfaces”

December 11 – 13, 2017

organized by

Pal Jedlovsky (Eszterházy Károly U, Eger) and Marcello Sega (U Vienna)

• **Monday, December 11, 2017**

09:00 – 09:30 **Opening & Registration**

09:30 – 09:40 **Welcome & Introduction**

09:40 – 10:10 **Edward Smith**

*A control volume study of the pressure tensor across a liquid-vapour interface*

10:10 – 10:40 **Patrice Malfreyt**

*Calculation of the interfacial tension from molecular simulations: a routine job ?*

10:40 – 11:00 *Discussion*

11:00 – 11:20 *coffee / tea break*

11:20 – 11:50 **Samuli Ollila**

*Inhomogeneous tension at biological lipid interfaces from molecular dynamics simulations*

11:50 – 12:30 **Pavel Jungwirth**

*Biological water or rather water in biology?*

12:30 – 12:50 *Discussion*

12:50 – 14:30 *lunch break*

14:30 – 15:00 **Ilpo Vattulainen**

*Phase behavior and dynamics of biomembranes under crowding*

15:00 – 15:30 **James L. Skinner**

*Water at air, lipid and surfactant interfaces - structure, dynamics, and spectroscopy*

15:30 – 15:50 *Discussion*

15:50 – 16:10 *coffee / tea break*

16:10 – 16:45 *Poster Session*

Dinner (19:30) at Restaurant “Mini”, Marchettigasse 11 (30-40 min from ESI)

- **Tuesday, December 12, 2017**

09:10 – 09:40 **Martin Lisal**

*Surface structures of binary mixtures of ionic liquids: insight from experiment, thermodynamics and molecular simulations*

09:40 – 10:10 **Miguel Jorge**

*Intrinsic analysis of ionic liquids at fluid interfaces*

10:10 – 10:30 *Discussion*

10:30 – 10:50 *coffee / tea break*

10:50 – 11:20 **Dominik Horinek**

*Octanol/water interfaces - from planar interfaces to surfactant-free microemulsions*

11:20 – 11:50 **David van der Spoel**

*Solvation free energies and other properties from liquid simulations*

11:50 – 12:10 *Discussion*

12:10 – 13:50 *lunch break*

13:50 – 14:30 **Ilan Benjamin**

*Water miscibility at the water/oil interface. molecular dynamics study of thermodynamics, dynamics and mechanism*

14:30 – 15:10 *Discussion*

15:10 – 15:30 *coffee / tea break*

15:30 – 16:45 *Poster Session*

- **Wednesday, December 13, 2017**

09:10 – 09:40 **Christoph Dellago**

*Bubble nucleation and the stability limit of water under tension*

09:40 – 10:10 **Maria Lbadaoui-Darvas**

*Unfolding the khler theory by atomistic molecular dynamics simulations*

10:10 – 10:30 *Discussion*

10:30 – 10:50 *coffee / tea break*

10:50 – 11:20 **Natalia Cordeiro**

*Probing the fluid behaviour near polymeric surfaces by molecular simulations*

11:20 – 11:50 **Laura Filion**

*Predicting phase behaviour of mixtures of active spherical particles*

11:50 – 12:30 *Discussion*

12:30 – 12:40 *Closing Word*

**All talks take place at the ESI, Boltzmann Lecture Hall!**