

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 **James L. Skinner**

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

15:00 – 15:20 **Discussion**

15:20 – 15:50 *coffee / tea break*

15:50 – 16:30 *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!