

7th MEETING ON MOLECULAR SIMULATIONS: *From simple fluids to chemical reactions*

HOTEL NH, Palma 42, Colonia Centro.

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Monday December 7th, 2015.

COMPUTER SIMULATION COURSE

10:00-14:00

PROTEIN -LIGAND SIMULATIONS. Cesar Millán, UAEM

7th MEETING ON MOLECULAR SIMULATIONS: *From simple fluids to chemical reactions*

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CONFERENCES

Thursday December 8th, 2015.

8:30-9:30 Opening Ceremony

CHAIRMAN: *Gustavo Chapela*

9:30-10:30 Julian Tirado Rives, Yale University, USA

*Molecular Monte Carlo simulations (and their surroundings):
developments and applications to systems of biological interest*

10:30-11:30 Humberto Saint Martin, UNAM, Mexico

*Using Molecular Dynamics to study phase equilibrium with direct
coexistence methods*

11:30-12:00 COFFEE

12:00-12:30 Jorge López Lemus, UAEM, Mexico

Surface tension of acetonitrile and aqueous solutions

12:30-13:00 Daniel Salgado Blanco, UAM-I, Mexico

Non-additive simple potentials for pre-programmed self-assembly

13:00-13:20 PICTURE OF ALL ATTENDEES

13:20-15:00 LUNCH (*)

CHAIRMAN: *Jorge Balmaseda*

15:00-16:00 Rolando Castillo, UNAM, Mexico

Disorder induced by capillary interaction between colloidal particles trapped at the air/water interface

16:00-16-30 COFFEE

16:30-17:00 Omar Castrejón González, Instituto Tecnológico de Celaya, Mexico

Rheology of complex fluids from Molecular Dynamics

17:00-18:00 Mathieu Bauchy, UCLA, USA

Stretched exponential relaxation of glasses at low temperature

18:00-20:00 POSTER SESSION (Sponsored by JCTC)



(*) Meal goes out on your own

Wednesday December 9th , 2015.

CHAIRWOMAN: *Susana Figueroa*

9:00-9:45 José Luis Rivera, UMICH, Mexico

The intramolecular pressure and the extension of the critical point's influence zone on the order parameter

9:45-10:45 Jeffrey J. Potoff, Wayne State University, USA

Development of State of the Art models and software for the prediction of vapor-liquid equilibria

10:45-11:15 COFFEE

11:15-12:00 José Antonio Moreno Razo, UAM-I, Mexico

Computer simulations of patchy particles

12:00-13:00 Nina Pastor, UAEM, Mexico

The role of a plant-specific binding pocket in information transfer pathways in profilins

13:00-14:00 Dmitry Matyushov, Arizona Stated University, USA

Theory and simulation of electron transfer in proteins