8th MEETING ON MOLECULAR SIMULATIONS: *From simple fluids to chemical reactions*

COURSES

Wednesday December 7th, 2016.

COMPUTER SIMULATION COURSES

10:00-13:00

ILLUSTRATING THE DRUG DESIGN PROCESS

Dr. Ponciano García Gutierrez, UAM-Iztapalapa

13:00 Lunch

14:30-17:30

MOLECULAR SIMULATIONS OF BIOLOGICAL SYSTEMS

Dra. Gloria Arlette Méndez Maldonado, UASLP

8th MEETING ON MOLECULAR SIMULATIONS: *From simple fluids to chemical reactions*

CONFERENCES

Thursday December 8th, 2016.

8:30-9:30 Opening Ceremony

CHAIRWOMAN: *Jacqueline Quintana Hinojosa*

9:30-10:15 Israel Cabeza de Vaca López, Yale University, USA

From Monte Carlo methods to drug discovery

10:15-11:00 G. Andrés Cisneros, University of North Texas, USA

Development and application of advanced potentials and QM/MM methods

11:00-11:30 COFFEE

11:30-12:15 Arturo Rojo Domínguez, Universidad Autónoma Metropolitana – Cuajimalpa, México

Molecular Simulations on Biological Systems

12:15-13:00 Héctor Jardón Valadez, Universidad Autónoma Metropolitana – Lerma, México

Molecular Simulation: a tool in Computational Biology applications

13:00-15:00 LUNCH

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CHAIRMAN: *G. Andrés Cisneros*

15:00-15:45 Julio Armas Pérez, Universidad de Guanajuato, Mexico

Phase Behavior of Lollipop-Shaped Hard Particles in Two Dimensions

15:45-16-15 COFFEE

16:15-17:00 Fernando del Río Haza, Universidad Autónoma Metropolitana – Iztapalapa, México

Free energy of the Square-Well fluid by Singular Value Decomposition

17:00-18:00 Red Temática de Teoría y Simulación Molecular Session

18:00-20:00 POSTER SESSION

20:00- Dinner conference

8th MEETING ON MOLECULAR SIMULATIONS: *From simple fluids to chemical reactions*

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Friday December 9th, 2016.

CHAIRWOMAN: *Ana Laura Benavides Obregón*

9:00-9:45 Meeting on Molecular Simulations Prize - Alejandro Gil-Villegas Montiel, Universidad de Guanajuato, Mexico

9:45-10:30 Francis W. Starr, Wesleyan University, USA

Applications of Coarse-Grained Molecular Modeling

10:30-11:00 COFFEE

11:00-11:45 Guillermo Ramírez Santiago, Instituto de Matemáticas-UNAM, Juriquilla, Mexico

Phase behavior of Langmuir monolayers with ionic molecular heads

11:45-12:30 Héctor Domínguez Castro, Instituto de Investigaciones en Materiales-UNAM, Mexico

Reactive Monte Carlo Method to study sorption of gases in solid surfaces

12:30-12:45 COFFEE

12:45-13:30 Manuel Martínez Piñeiro, Universidad de Vigo, España

Molecular modeling of carbon dioxide hydrates: comparison of different approaches

13:30-14:30 Winners of the Poster Session Prize