9th MEETING ON MOLECULAR SIMULATIONS: *From simple fluids to chemical reactions*

INDUSTRIAL ISSUES

Wednesday December 6th, 2017.

14:00 - 16:00

ENERGY STORAGE

Dr. Edgar Núñez Rojas – Conacyt-UAMI
Dr. Guadalupe Ramos Sánchez – Conacyt-UAMI

16:00 - 18:00

DRUG DESIGN

Dr. Rafael Arturo Zubillaga Luna
Dr. Rodolfo Pinal – Universidad de Purdue
Dr. Ponciano García Gutierrez – UAMI
Dra. Lena Ruíz Azuara – Facultad de Química

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Thursday December 7th, 2017.

8:30 - 9:30 Opening Ceremony

CHAIRWOMAN: *Ana Laura Benavides*

9:30 - 10:20 Gustavo Chapela Castañares, UAM-Iztapalapa, Mexico

Programmable Matter

10:20 - 11:10 Gren N. Patey, British Columbia University, Canada

The Birth and Growth of Salt Crystals: Insights from Molecular Dynamics Simulations

11:10 - 11:40 COFFEE

11:40 - 12:20 Marco Tulio Gallo Estrada, Tecnológico Nacional de México, Cd. Juárez, Chihuahua, Mexico

Determination of free energy reaction pathways using imidazolium ionic liquids as catalysts by molecular simulations

12:20 - 13:00 María del Alba Pacheco Blas, IIM-UNAM, Mexico

Surfactant molecules to promote removal of cadmium ions from solid surfaces: A complementary experimental-simulational study

13:00 - 13:30 attendees picture (Zócalo)

13:30 - 15:30 LUNCH (NH hotel)

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CHAIRMAN: *Héctor Domínguez Castro*

15:30 - 16:10 Francisco Sastre, Universidad de Guanajuato. Mexico

A microcanonical-ensemble computer simulation method for discrete potential fluids

16:10 - 16:40 COFFEE

16:40 - 17:20 Pedro Orea, Instituto Mexicano del Petróleo, Mexico

Interfacial Properties of Simple Fluids

17:20 - 18:00 Carlos Ignacio Mendoza Ruiz, IIM-UNAM, Mexico

Incomplete capsid formation: coarse-grained and elastic modeling

18:00 - 20:00 POSTER SESSION

20:00- Dinner conference (NH hotel)

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Friday December 8th, 2017.

CHAIRMAN: *Humberto Saint-Martin*

9:00 - 9:50 Rodolfo Pinal, Purdue University, USA

New platform for the design and manufacture of patient-centric pharmaceuticals

9:50 - 10:30 Marco Heinen, Universidad de Guanajuato, Mexico

The Hard Sphere Fluid in 1.68 Dimensions

10:30 - 10:50 COFFEE

10:50 - 11:30 Jorge Lozano-Aponte, BUAP, Mexico

Study of interactions between LPS-derivatives and the dimeric TLR4/MD-2 receptor complex by Molecular Dynamics simulations

11:30 - 12:10 Annia Galano Jiménez, UAM-Iztapalapa, Mexico

Rational Design of Multifunctional Antioxidants

12:10 - 13:00 Andres Jaramillo-Botero, California Institute of Technology, USA

Large-Scale, Quantum-based Non-Adiabatic Molecular Dynamics Simulation of Materials in Extreme Conditions

13:00 - 13:20 COFFEE

13:20 - 14:20 Winners of the Poster Session Prizes