

11th Meeting on Molecular Simulations:

From simple fluids to chemical reactions.

PROGRAM

November 14, 2019

15:00 - 17:00

COCRYSTALS

Juan Manuel Germán Acacio

Herbert Höpfl

Frank José Salas Sánchez

17:00 - 19:00

ROOM TEMPERATURE IONIC LIQUIDS

Natalya V. Likhanova

Zaira J. Domínguez Esquivel

José Alejandro

November 15, 2019

08:30 - 09:10 **Opening ceremony**

CHAIRMAN: **Humberto Saint-Martin Posada**

9:10 - 10:10 *Andrés Cisneros (webinar) - Desarrollo y Aplicaciones de AMOEBA-I*

University of North Texas, USA

10:10 - 11:10 *Jeffrey Potoff (webinar) - To be announced*

Wayne State University, USA

11:10 - 11:30 **COFFEE BREAK**

11:30 - 12:30 *Jose Nuno Canongia Lopes (webinar) - To be announced*

Universidade Técnica de Lisboa, Portugal

12:30 - 13:00 *Minerva González Melchor* – Dielectric behavior of water within a surfactant bilayer: a molecular dynamics study

Instituto de Física, BUAP, Mexico

13:00 - 13:15 **Attendees picture**

13:15 - 15:00 **LUNCH (Hotel NH)**

CHAIRMAN: **Héctor Domínguez Castro**

15:00 - 15:30 *Oswaldo de Melo Pereira* - Interfacial strain defines the self-organization of epitaxial MoO₂ flakes and porous films on sapphire: experiments and modelling

Facultad de Física, Universidad de La Habana, Cuba

15:30 - 16:00 *Angélica Estrella Ramos Peña* - Weak interactions in DNA: a DFT study in CpG-island-like chains

Instituto de Investigaciones en Materiales, UNAM, Mexico

16:00 - 16:30 **COFFEE BREAK**

16:30 – 17:00 **Javier Carmona Espíndola** - Constrained Dipole Moment Density Functional Theory for Charge Distributions in Force Fields for the Study of Molecular Fluids
CONACyT-UAM Iztapalapa, Mexico

17:00 - 17:30 **Marco Vinicio Velarde Salcedo** - Low Hydroxylated Fullerenes: Stability, Thermal Behavior, and Vibrational Properties
Facultad de Ciencias, UAEM, Mexico

17:30 - 18:00 **César Millán Pacheco** - Pharma-Dock, another docking server based on free software
Facultad de Farmacia, UAEM, Mexico

18:00 - 20:00 **POSTER SESSION**

20:30 - **Award-winnings and dinner conference Meeting on Molecular Simulations Award Announcement of winner posters (Restaurant Quereres Sabor Mexicano)**

November 16, 2019

CHAIRWOMAN: Ana Laura Benavides Obregón

9:00 – 09:30 **Eduardo Villareal Ramírez** - An undiscovered code in the intrinsically disordered proteins: Phosphorylation as control of ligand binding and protein structure
Facultad de Odontología, UNAM, Mexico

9:30 – 10:30 **Iván Ortega Blake** – Nanodomain formation in the lipidic bilayer, origin, modulation and biological relevance
Instituto de Ciencias Físicas, UNAM, Mexico

10:30 - 11:00 **COFFEE**

11:00 - 11:30 **Manuel Martínez Jiménez** - Aqueous solutions of methanol, ethanol and 1-propanol: numerical simulations of the liquid phase and liquid-vapor coexistence using refined molecular models
UAM Iztapalapa, Mexico

11:30 - 12:00 **Francisco Alarcón Oceguera** - Biofilms under hydrodynamic stress
Universidad de Guanajuato, Mexico

12:00 – 12:50 **Chantal Valeriani** - The role played by interactions in the assembly of active colloids
Universidad Complutense de Madrid, Spain

12:50 - 13:15 **COFFEE**

13:15 - 14:00 **Winners of the Poster Session Prizes**

