

**10th MEETING ON MOLECULAR SIMULATIONS: *From simple fluids to chemical reactions***

**INDUSTRIAL ISSUES**

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**Thursday November 8th, 2018.**

**15:00 - 17:00**

**ENERGY STORAGE**

**Jorge Gabriel Vázquez Arenas**

**Marcelo Galván Espinosa**

**José R. Alejandro Ramírez**

**17:00 - 19:00**

**DRUG DESIGN**

**Ravi Radhakrishnan**

**Marlet Martínez Archundia**

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**Friday November 9th, 2018.**

**CHAIRWOMAN: Ana Laura Benavides Obregón**

**9:00 - 9:50 Susana Figueroa Gerstenmaier - UG, Mexico**

*Molecular simulations of adsorption of gases in polymeric materials*

**9:50 - 10:40 Badhin Gómez Valdez - Universidad Católica de Santa María, Perú**

*Evaluation of the effect of the charges model in the OPLS-AA force field for ionic liquids, which best reproduces its properties in liquid phase conditions*

**10:40 - 11:10 COFFEE**

**11:10 - 11:40 Alexander Pérez de la Luz - UAM-Iztapalapa, Mexico**

*Force Field Parameterization via Atoms-in-Molecules*

**11:40 - 12:10 María del Rosario Eustaquio Armenta - IF, BUAP, Mexico**

*Diffusion in 2D ionic fluids*

**12:10 - 12:50 Alejandro Ramírez Solís - Centro de Investigación en Ciencias, UAEM, Mexico**

*Theoretical studies of the epsilon and dzeta high pressure phases of solid oxygen. Electronic properties, relative stability, finite temperature effects and the transition to the superconducting dzeta phase*

**12:50 - 13:00 attendees picture**

**13:00 - 15:00 LUNCH (hotel)**

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**CHAIRWOMAN: Arlette Méndez Maldonado**

**15:00 - 15:50 Ravi Radhakrishnan - University of Pennsylvania, USA**

*Multi-scale Modeling of Proteins and Membranes*

**15:50 - 16:20 COFFEE**

**16:20 - 17:00 Marlet Martínez Archundia - IPN, Mexico**

*Structural studies of G protein coupled receptors by using Molecular dynamics simulation and docking studies*

**17:00 - 17:40 Laura Domínguez Dueñas - FQ, UNAM, Mexico**

*Characterizing  $\gamma$ -secretase, responsible for the generation of amyloid- $\beta$  peptides*

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

**20:00 - Award-winnings and dinner conference**

**Meeting on Molecular Simulations Award**

**Announcement of winner posters**

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**Saturday November 10th, 2018.**

**CHAIRMAN: Humberto Saint-Martin Posada**

**9:00 - 9:50 Meeting on Molecular Simulations 2018 awarded**

**9:50 - 10:30 Illich Argel Ibarra Alvarado - IIM, UNAM, Mexico**

*Confinement of polar molecules to enhance CO<sub>2</sub> capture in MOFs*

**10:30 - 10:50 COFFEE**

**10:50 - 11:20 César Iván León Pimentel - ICF, UNAM, Mexico**

*Aqueous solvation of divalent cations and acids through Born-Oppenheimer molecular dynamics simulations and polarizable force fields*

**11:20 - 12:00 Orlando Guzmán López - UAM-Iztapalapa, Mexico**

*Self-assembly of micro-capsules formed by nanoparticles via liquid crystal sorting*

**12:00 - 13:00 Andrij Trokhymchuk - Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine**

*Hard-core colloids under confinement: what can be learn from computer simulations*

**13:00 - 13:20 COFFEE**

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