



**IBER 2023****Wednesday, 6 September 2023****Oral communications (12:00 - 13:00)**

time	[id] title	presenter
12:00	[4] Photodeactivation mechanisms of graphene quantum dots	Dr GÓMEZ RODRÍGUEZ, Sandra
12:15	[5] Charged nanosilicate Clusters and their Interaction with Oxygen: Astronomical Relevance	Mr MARIÑOSO GUIU, Joan
12:30	[11] Proton diffusion in a benchmark entangled hydrogen bonding network	Prof. MARTÍNEZ-HAYA, Bruno
12:45	[22] Simulation of Pm-Like Bismuth Spectra in an EBIT	MARQUES, J. P.

**Oral communications (16:00 - 16:30)**

time	[id] title	presenter
16:00	[33] RAMAN THERMOMETRY OF CONFINED GAS MICRO-FLOWS	Dr FERNÁNDEZ, José M.
16:15	[41] The Plasma Window as a Vacuum-Atmosphere Interface for Measurements of Stellar Neutron-Induced Reaction Cross Sections	RUIMI, Ophir

**Oral communications (17:45 - 18:30)**

time	[id] title	presenter
17:45	[29] Variational principle to regularize machine-learned density functionals	DEL MAZO SEVILLANO, Pablo
18:00	[99] Determination of the absolute primary scintillation yield of pure krypton	Mr MANO, Rui Daniel P
18:15	[61] Ultrafast X-ray and optical studies of charge carries dynamics in colloidal quantum dots	Prof. GAWELDA, Wojciech

# Thursday, 7 September 2023

## Oral communications (12:00 - 13:00)

time	[id] title	presenter
12:00	[19] Exploring space chemistry: quantum spectroscopic characterization of Ng-containing molecules through machine learning algorithms.	Ms MONTES DE OCA ESTEVEZ, María Judit
12:15	[76] Photophysics of protonated vanillin in the gas phase: a laser action spectroscopy and theoretical approach	GUTIÉRREZ QUINTANILLA, Alejandro
12:30	[39] Measuring physical quantities of CO <sub>2</sub> by Raman spectroscopy	ALVAREZ, Carlos
12:45	[23] Using a 125 $\mu\text{m}$ thick COBRA to increase the light yield of He-CF <sub>4</sub> gas mixtures	ROQUE, Rita

## Oral communications (16:00 - 16:45)

time	[id] title	presenter
16:00	[38] TRIGGERING EXCITED STATE DYNAMICS IN GRAPHENE QUANTUM DOTS: THE ABSORPTION SPECTRUM OF CORONENE AND CIRCUMCORONENE	MARTÍN SANTA DARÍA, Alberto
16:15	[45] Benzimidazole: One molecule - two photoreactions	Dr REVA, Igor
16:30	[50] Interstellar detection of carbonic acid (HOCOOH) at last	SANZ NOVO, Miguel

## Oral communications (18:00 - 19:00)

time	[id] title	presenter
18:00	[34] Exploring the Interaction of Endogenous Therapeutic Peptides with Lipid Membranes: Insights from Biased calculations.	CONDE TORRES, Daniel
18:15	[81] THCOBRA detector performance in mixtures of Kr/Xe mixtures	DAS NEVES DIAS CARRAMATE, Lara Filipa DAS NEVES DIAS CARRAMATE, Lara Filipa
18:30	[43] Time evolution of natural orbitals in ab initio molecular dynamics	PIRIS, Mario
18:45	[64] Atomic Calculations and Data Using the MultiConfiguration Dirac-Fock General Matrix Elements (MCDFGME) code	PINHEIRO, Daniel

# Friday, 8 September 2023

## Oral communications (12:00 - 13:00)

time	[id] title	presenter
12:00	[16] Ultralong-range Cs-RbCs Rydberg molecule: non-adiabaticity of dipole moments	MELLADO-ALCEDO, David
12:15	[107] The PISA Photosensor for Multi-Ton Rare Event Detectors	Dr BERNARDES MONTEIRO, Cristina M
12:30	[51] Non-Covalent Interactions in Carbon Dioxide Clusters: Comparison Between the Thiophenol-CO <sub>2</sub> and Benzylmercaptan-CO <sub>2</sub> Dimers Using Microwave Spectroscopy	Ms LI, Wenqin
12:45	[35] Status and recent results of the XENONnT experiment	PERES, Ricardo

## Oral communications (16:10 - 17:10)

time	[id] title	presenter
16:10	[26] A new analytical potential energy surface for (H <sub>2</sub> <sup>+</sup> )He cluster	HERNÁNDEZ ROJAS, Javier
16:25	[37] Investigating the Catalytic Mechanism of β-Cyclodextrin Dimer in Previtamin D <sub>3</sub> Isomerization	Dr FERRO-COSTAS, David
16:40	[15] The cationic lithium dimer solvated in He clusters: Molecular Dynamics Simulations.	VILLARREAL, Pablo
16:55	[48] Effect of the intersystem crossings in the S <sub>0</sub> +H <sub>2</sub> reaction	ZANCHET, Alexandre

## Oral communications (18:00 - 19:15)

time	[id] title	presenter
18:00	[44] Computational Ingredients to Model Biological Processes	NOGUEIRA PÉREZ, Juan Jose
18:15	[63] Unveiling the Aggregation Patterns of Curcumin and Piperine Mixtures in different Polar Media: A Molecular Dynamics Investigation	R. C. SANTOS, Joana
18:30	[28] Understanding the formation of aromatic compounds in the interstellar space	NOT SUPPLIED, CASTIÑEIRA REIS MARTA
18:45	[40] Improvement and benchmarking of atomic data for kilonova modeling	LEITÃO, Luís
19:00	[24] Exploring the secondary structure of Host Defense Peptides in their biological environment. A Molecular Dynamics approach.	SUÁREZ-LESTÓN, Fabián