Poster session 1. Bio1 - Carles Curutchet

Poster	Title	Speaker
PA1	Towards the Computational-Assisted Design of Enzymes for the Recycling of Synthetic Polymers	Vicent Moliner
PA2	Rules governing metal coordination in Aβ-Zn(II) complex models from quantum mechanical calculations	Julen Aduriz Arrizabalaga
PA3	Influence of metal binding on the conformational landscape of neurofilament peptides.	David Silva Brea
PA4	Understanding the origin of the L-glutaminase side-activity of L-asparaginase	Leslie Sánchez
PA5	Computational approaches to find the hidden phosphate hydrolysis intermediate in ATPase p97	Judit Katalin Szántó
PA7	Electronic structure and intermolecular interactions of antichagasic peptides as cruzipain inhibitors: A DFT study	Catalina Soriano Correa
PA8	Loop Opening and Closing Dynamics and Reactivity in Orotidine 5′-Monophosphate Decarboxylase	Johanna Schillings
PA9	Computational study of the chemiexcitation of a dioxetane derivative of melanin and its implications for DNA damage	Juliana Cuéllar Zuquin
PA10	Modelization of Synaptic Vesicles to study the Effect of Glycation on Dopamine Transport	Juan Frau Munar
PA11	Exploring Small Molecule Interactions with DNA: Implications in DNA Damage and Cancer Treatment	Julia Arnanz Sebastián

Poster session 2. Bio2 - Katarzyna Świderek

Poster	Title	Speaker
PA12	Unraveling the Activation of EP4 Receptor by Prostaglandin E2	Álex Pérez Sánchez
PA13	Role of the Active Site Lysine Residue on FAD Reduction by NADPH in Glutathione Reductase	Jenner Bonanata
PA14	Computational Analysis on the conversion of a Metallo-Oxidase into a Laccase by directed evolution experiments	Laura Masgrau
PA15	Electrophilic Nitroalkenes of Unsaturated Fatty Acids (NO2FA) as Modulators of Protein Function: the FABP4-PPARγ Axis and PGHS-2 (COX-2) as Targets	E. Laura Coitiño
PA16	Phosphorated indoquinoline derivatives as Topoisomerase I inhibitors	Elena Formoso Estensoro
PA17	Force Field Parameterization of the Firefly's Bioluminescent Chromophores	Henar Mateo de la Fuente
PA18	Computational Study of Ion Conduction through ORF3a Viroporin by Molecular Dynamics	Nuria Anguita Ortiz
PA19	Computational Characterization of the Interactions between Anticancer Drugs and Lipid Membranes	Lorena Ruano de Domingo
PA20	Structural Dynamics and Substrate Interactions in Glycyrrhiza glabra C-Glycosyltransferase: A Computational Approach to Elucidate Catalytic Complexes	Fernanda Mendoza
PA21	Time-evolution of Non-covalent Interactions in Spontaneous Binding Molecular Dynamics Simulations	Cristina Berga
PA22	Theoretical Eumelanin Dimer Models - Towards Unravelling The Structure of Melanin	Anju Manickoth

Poster session 3. HetCat1 - Josep Manel Ricart

Poster	Title	Speaker
PA23	Insights into metal-catalysed reverse Water-Gas Shift reaction through reactive force fields	Gerard Bru Garcia
PA24	Choline-based Deep Eutectic Solvents: one force field to rule them all?	Elixabete Rezabal
PA25	Solvation effects in the reaction profiles of the hydrogenation of Nitrobenzene to Aniline catalyzed on Palladium	Javiera Herrera Escalona
PA26	Theoretical and experimental study of propane dehydrogenation on Pt single-atom on different supports.	Jie Pan
PA27	Exploring Cholinium-Based Catalysts for PET Recycling: Understanding the Role of Ethylene Glycol Solvent	Diana Bura
PA28	Computational study of the Lewis acid and base-catalyzed zwitterionic ring-expansion polymerization (ZREP) of monosubstituted epoxides	Xuban Gastearena
PA29	Hydrogen Tunneling in Catalytic Hydrolysis and Alcoholysis of Silanes	Jon M. Matxain
PA30	Multiscale approach for CO2 hydrogenation on Silicalite-encapsulated Ru atoms	Manuel Antonio Cánovas Montes
PA31	A comparative kinetic study of the CO2 hydrogenation reaction on Ni(111) surface: Microkinetic Modeling vs. kinetic Monte Carlo simulations	Alejandro Gracia Gil
PA32	CO Poisoning Resistant Pt Catalysts Design through Ge Alloying	Jose M. Mercero
PA33	Employing Symmetric XB-Based Catalytic Scaffolds for Ring-Opening Polymerisation	Nika Melnyk

Poster session 4. ML -Jordi Carbó

Poster	Title	Speaker
PA34	Enzyme engineering for polyethylene terephthalate (PET) biodegradation through machine learning and electrostatic properties.	Rafael Garcia Meseguer
PA35	MODA: a quantum-inspired representation designed for predicting intermolecular properties by means of Machine Learning	Raul Santiago Piera
PA36	Smooth Sailing in Rough Waters of Excited States with Machine Learning	Štěpán Sršeň
PA37	Multiscale simulations with machine learning molecular potentials	Kirill Zinovjev
PA38	Using Inverse Molecular Design and Explainable Machine-Learning to Design and Understand Nonlinear Optical Molecular Switches	Eline Desmedt
PA39	Predicting the pKa of opioids: A machine learning approach	Guillermo García Díez
PA40	Towards Efficient Water Oxidation Catalysts: Insights from DFT and Data Analysis	Mario Villares Cañón
PA41	Enhancing thermoelectric efficiency in Co-free skutterudites: combining experiments, ab-initio calculations and machine learning	Jose J. Plata Ramos
PA42	Reconciling theory and experiments in the analysis of lattice thermal conductivity: the Cu-based sulvanites	Antonio M. Márquez
PA43	ROBERT: Bridging the Gap between Machine Learning and Chemistry	David Dalmau
PA44	FAIR reaction mechanisms through ioChem-BD	Diego Garay Ruiz

Poster session 5. Organic Reactivity - Xavier López

Poster	Title	Speaker
PA45	An unexpected problem of astrochemical significance and a healing strategy	Javier Dominguez Calvo
PA46	Insights on the Energy Dissipation Process Released by the Formation of Formamide on Interstellar Water Ice Surfaces	Berta Martínez i Bachs
PA47	Ionization of atmospheric relevant molecules using O2- superoxide anion	Mariana Leiferman Tamames
PA48	Heterogeneous astro-catalysis. Insights to the Fe single-atom and nano-cluster catalysis in space from quantum chemical simulations	Gerard Pareras
PA49	Investigating CO2 Formation on Interstellar Water Ice: A Computational Study	Harjasnoor Kakkar
PA50	Optimising Hypervalent Iodine Catalysts: Halogen-Bonding Strengths Explored via Michael-Addition	James O'Brien
PA51	Determining the ambimodality of chemical reactions	Jordi Soler
PA52	Time Independent Close-Coupling Approach to Non-Reactive H3+ + H Collisions	Daniel Félix González
PA53	Fullerene Reactivity: A Comprehensive Study of the Bingel-Hirsch Reaction	Daniel Torrens González
PA54	Mechanistic Insights Behind the Divergence in Outcomes in Ball-Milling and Solution Reactions of Fullerenes	Eduardo García-Padilla

Poster session 6. PhotoChem1 - Josep Maria Bofill

Poster	Title	Speaker
PA55	Towards Understanding the Mechanism of Magnetoluminescence in Triarylmethyl-Based Diradicals	Fatemeh Mamusi
PA56	Excitation of porphyrin photosensitizers by accelerated protons	Judit Gálvez
PA57	Modelling Photoinduced Damage and Control of Biological Systems	Juan José Nogueira Pérez
PA58	Photoswitchable control of the 5-HT2AR signal transduction	Vito Federico Palmisano
PA59	On the photophysics of cyclometalated Ir(III) complexes: the B3LYP and PBE0 functionals at comparison	Iván Soriano Díaz
PA60	Mapping the Potential Energy Surfaces of Excited States in Organic Compounds: Understanding Their Role as Photosensitizers.	Anna Cholewinska
PA61	Electronic structure of mononuclear iron phthalocyanine complexes in matrix isolation spectroscopy: experiment challenges theory	Carlos Jimenez-Muñoz
PA62	Adjusting UV-Vis Spectrum of Alizarin by Insertion of Auxochromes	Zahra Noori
PA63	Molecular dynamics simulations for triazoles group of fungicides: First steps to simulate tandem mass spectrometry predictions.	Sergio Pérez Tabero
PA64	Formation of Excited States in the Decomposition of Dioxetane via Mixed Reference SF-TDDFT NAMD	Juan Carlos Roldao

Poster session 7. ElStructure - Daniel Reta

Poster	Title	Speaker
PA65	Spin-Adapted and Spin-Purified Stochastic GASSCF	Oskar Weser
PA66	Exploring INVEST molecules with Piris natural orbital functionals and the extended random phase approximation.	Juan Felipe Huan Lew Yee
PA71	Measures of Electron Correlation for Multireference Diagnostics	Eloy Ramos-Cordoba
PA67	Development of electron correlation indicators	Markel Ylla
PA68	Excitonic Renormalization: A novel fragmentation scheme for Modular Large-scale ab initio Electronic-structure Calculations	Marco Bauer
PA69	Open Subsystem-Based Partition of Molecular Energies into Resonance Structure-Resolved Contributions	Diogo Rodrigues
PA70	DFA calibration from highly-accurate energies and densities at different correlation regimes	Rubén R. Ferradás
PA72	Pushing the Limits of Accuracy: MP2 Theory Enhanced by Smeared Electron Density Orbitals	Danjo De Chavez
PA73	Dense-Sparse Quantum Monte Carlo Algebraic Diagrammatic Construction and Importance Ranking	Adem Halil Kulahlioglu
PA74	Recent Progress in Stochastic Complete Active Space Second-Order Perturbation Theory	Arta Safari
PA75	Beyond the quasiharmonic approximation: a simple approach to quasiparticle thermodynamics	Ernesto Blancas Jimenez

Poster session 8. Materials1 - Toni Rodriguez-Fortea

Poster	Title	Speaker
PA76	Donor-Acceptor Supramolecular Complexes Based on Carbon Buckybowls of Increasing Size: A Theoretical Study into the Charge-Separation Rate Constants	Raquel Rubert Albiol
PA77	Impact of the peripheral functionalization on electronic properties of Spirobifluorenes (SBFs)	Julia Portela Pino
PA78	Anisotropic Pressure of Nanoconfined Water within Narrow Graphene Slit Pores	Sergi Ruiz-Barragan
PA79	Kinetic Monte Carlo simulations of transport dynamics in polymer-based memristive devices	Gerliz Gutierrez Finol
PA80	Metal-cage interaction in Endohedral Mono-Actinidofullerenes	Khaoula Merimi Aqlane
PA81	Theoretical study on the intercalation of organic compounds in clays (montmorillonite) for bioavailability control.	Alexander Pérez de la Luz
PA82	A multi-level theoretical approach for morphology, dynamic disorder and charge transport characterization of hole-transporting materials	Alberto Fernández Alarcón
PA83	The Emerging 2D Boron Chemistry	Josep M. Oliva Enrich
PA84	Electron-spin relaxation in boron-doped graphene nanofragments	Roberto A. Boto
PA85	Pushing the Limits of First Principle-Based Approaches to Characterize Organic Semiconductor Thin Films: Modeling Photo Physical Effects of Complex Crystal Packings and Blends	Maximilian Asbach

Poster session 9. Bio3 - Maite Roca

Poster	Title	Speaker
PB1	Deciphering the molecular mechanisms of reactive metabolite formation in the mechanism-based inactivation of cytochrome p450 1B1 by 8-methoxypsoralen and assessing the driving effect of phe268.	Al Mokhtar Lamsabhi
PB2	Understanding the Molecular Structure of Choline Geranate (CAGE) in Water: Insights from Molecular Dynamics Simulations	Mikel Loizate Gutierrez Canas
PB3	Reactivity and Inhibition of Arginine Gingipain B. A promising target for the treatment of Alzheimer's disease.	Maite Roca
PB4	An unusual His/Asp acid/base dyad in glycosidase catalysis. Insight from QM/MM MD simulations.	Mert Sagiroglugil
PB5	Molecular mechanism and determinants for the unique specificity of the Akkermansia muciniphila sialidase GH181	Marina Corbella Morató
PB6	Bio-degradation of Polyurethanes by Candida Antarctica Lipase B (CALB)	Carmen Ramos Vellón
PB7	Mechanistic Insights into the Anticancer PtIV Prodrugs Extracellular Activation: Reduction to Cisplatin by Cysteine and Homocysteine	Fabiana Salazar
PB8	Environment effects change FRET distributions in a fluorophore-tagged disordered protein	Daniel Gonzalo Palao
PB9	Alteration of Cardiac Titin Protein Mechanical Properties by Glycation	Rodrigo Casasnovas Perera
PB10	Exploring the Reaction Mechanisms of hASNase3 and gpASNase1 through Multiscale Simulations	Jose Javier Ruiz Pernía
PB11	How ATP hydrolysis drives conformational changes in a biomolecular motor: The case of Zika NS3 helicase	Adrián García Martínez

Poster session 10. PhotoChem2 - Maria Besora

Poster	Title	Speaker
PB12	Disclosing the role of oxo substitution in the photochemistry of purines and pyrimidines: implications for prebiotic chemistry	Inés Corral
PB13	Photochemistry upon charge separation in triphenylamine derivatives	Letao Huang
PB14	Free Energy Perturbation Theory for Triplet Energies Determination in DNA	Miriam Navarrete Miguel
PB15	CASPT2 determination of the ClOOCl UV/Vis Absorption Spectrum and Photodissociation Channels to Accurately Quantify their role in the Ozone Depletion Mechanisms	Cristina López Cava
PB16	Light response of Synthetic DNA: exploring the photophysics of Hachimoji nucleobases.	Marta Ibañez-deLuis
PB17	On the control of the ultrafast photodeactivation mechanism in [Fe(bpy)3]2+	Marc Alias
PB18	Theoretical exploration of azaborine derivatives suitable for MOST systems	Adrian Müller
PB19	Calculation of Dark Excited States in Conjugated Organic Molecules	Begoña Milián Medina
PB20	Light-triggered dissociations of sulfur- and mercury-containing compounds	Antonio Francés Monerris
PB21	Ultrafast photogeneration of a metal-organic nitrene from 1,1′-diazidoferrocene	Frederik Scherz
PB22	Unraveling Cryptophyte Photoacclimation: Insights from Multiscale Computational Studies on Pigment-Protein Antenna Complexes	Renato D. Cunha

Poster session 11. HetCat2 - Josep Maria Oliva

Poster	Title	Speaker
PB23	Modeling pH-Dependent Properties of Microbial Rhodopsins	Darío Barreiro Lage
PB24	Assessment of MXenes as photocatalytic materials for water splitting	Carmen Sousa
PB25	Photocatalytic OER on Semiconductors: Mechanistic Insights from DFT	Denis Diatlov
PB26	Evaluating electrochemical cross-electrophile coupling promoted by overcharge protection	Marina Díaz Ruiz
PB27	H2O – iron oxide-based nanoparticles interphase by means of DFT calculations	Adenilson Sousa Silva
PB28	DFT study to uncover regioselectivity in carboxylate-assisted C-H activation of NHC-Pd complexes	Edmond Apaloo Messan
PB29	Multi-FLPs and cooperative effect : study of the capture of CO2 by LAxLBy-doped nanographenes.	Maxime Ferrer
PB30	Understanding dynamic catalyst-electrolyte interfaces to improve eCO2RR	Enric Ibáñez Alé
PB31	High-throughput discovery of catalysts for the hydrogen economy through machine learning	Valentin Vassilev Galindo
PB32	Study of Pt8 in gas phase. Ab-initio molecular dynamics to address fluxionality in metal nanoclusters	Ramon Bergua
PB33	DFT study of the Suzuki-Miyaura cross-coupling allylation using a Pd-Fe heterobimetallic MOF catalyst	Pablo Gómez-Orellana Seguín

Poster session 12. HomoCat - Kirill Zinovjev

Poster	Title	Speaker
PB34	Exploring the landscape in copper(I)-catalyzed oxidative addition of aryl and alkyl bromides	Jesús Jover
PB35	Exploring the Electrochemical Kinetics of Water Oxidation Using Polyoxometalate Catalysts	Mireia Segado Centellas
PB36	A look into the stereoselectivity in the formation of interstellar sugar precursors on amorphous solid water: from vinyl alcohol to (Z)-1,2-ethenediol	Juan Carlos del Valle Morales
PB37	Resolving the mechanism for H2O2 decomposition over Zr and Ti catalysts	Jordi Puiggalí Jou
PB39	DFT Simulation of Complex Reaction Networks for Solving Aqueous Speciation of Polyoxometalates	Jordi Buils Casasnovas
PB40	Thioether-containing tertiary aldehyde radicals for controlled CO release and thiol decaging: a DFT study	María Milagros Muriel Olaya
PB41	Mechanistic Studies of Co(I) catalysed [2+2+2] cycloadditions to yield pyridine derivatives	Victor Polo
PB42	DFT study of the aerobic oxidation of lignin models using a Vanadium (V) complex	Laura Sánchez Guirao
PB43	Modelling of Guest-Binding by Molecular Pincers	Gantulga Norjmaa
PB44	Catalytic Alcohol Coupling Reaction through Borrowing Hydrogen Process	Núria Alsina Pla

Poster session 13. Magnetism - Ramon Sayos

Poster	Title	Speaker
PB45	Computational assisted design of Spin-Crossover systems with tailored transition temperatures: From molecules to Metal-Organic Cages	Jordi Cirera
PB46	Co2+ and Cu2+ magnetic porphyrin dimeric rings mechanically-bonded around carbon nanotubes for quantum technological applications	Rocío Sánchez de Armas
PB47	Analysis of super exchange pathways in μ-oxo bridged dinuclear complexes	Justin Krampe
PB48	Understanding The Magnetic Nature of Bare MXenes in their Electronic Ground State	Néstor Mauricio García-Romeral González
PB49	Computational study of Spin-Crossover systems Embedded in Carbon Nanohoops and its effects on the Transition Temperature	Arnau Garcia Duran
PB50	Towards Polyradicals: A Planar and Fully π- Conjugated Organic Tetraradical(oid)	Sergi Betkhoshvili
PB51	Spin-Adapted Effective Hamiltonians for S_local > ½ Polynuclear Magnetic Clusters	Arta Safari
PB52	Insights on Molecular Qubit Spin Relaxation: Hyperfine Coupling Role	Joan Cardona Olives
PB53	Electronic and magnetic properties of triangulene monomer and its oligomers	Alicia Omist Galvez
PB54	Accurate and efficient multi-reference electronic structure calculations with spin-orbit couplings for lanthanide ions	Rahul Jingar
PB86	Permutation symmetry in spin adapted many-body wave functions	Maru Song

Poster session 14. MolProp - Xavier López

Poster	Title	Speaker
PB55	Analysis of Acene Cation Excited States using ADC and TDDFT	Anna Marleen Weidlich
PB56	Charge-Transfer States in Action: Impact on Optical Behaviors and Exciton Diffusion in Molecular Aggregates	Jesús Cerdá
PB57	Understanding vibrational temperature effects on Mössbauer parameters using a sampling approach	Niklas von Rhein
PB58	Computational study of aromaticity with electron delocalization indices.	Ander Aleson Gurruchaga
PB59	Theoretical study of structural and electronic trends of sulfonylurea herbicides family	Mónica Valentín Rodríguez
PB60	Should electronic delocalization be associated with aromaticity? The case of c-P6•T6^6+ .	Luis Soriano-Agueda
PB61	A multiscale approach for vertical excitations of organic molecules in solution	Matteo Rinaldi
PB62	Q-ADC(2): The Second-Order Algebraic Diagrammatic Construction Scheme for the Polarization Propagator by Quadrature	Antonia Papapostolou
PB63	Acetonitrile Real Gas Phase Behavior from quasi-ideal gas to nanodroplets: A Microscopical View	Enrique Sánchez Marcos
PB64	An automated computational strategy to efficiently account for the counterion effect in solution. Application to the electronic structure of polyoxometalates	Albert Masip-Sánchez
PB65	Simulation and Conformational studies of Maleic Anhydride Tetramer: An Exploration using Umbrella Sampling and GaMD	Abhishek Anil Nair

Poster session 15. Characterization - Josep M. Poblet

Poster	Title	Speaker
PB66	A Quantum Chemical Topology perspective on the fluoride – teflate analogy	Julen Munárriz
PB67	How electrons still guard the space	Daniel Barrena Espés
PB68	A Quantum Chemical Topology study of Pyramidanes	Lucía Vidal Aguilar
PB69	Ion-pair interactions in σ-alkane complexes in the solid state: a comparison of wavefunction and density-based methods	Carlos Martin Fernandez
PB70	Surely you're joking Mr. Lewis!: Double quartets, not octets.	Ángel Martín Pendás
PB71	Evaluating Aromaticity in Large Conjugated Systems with Hilbert-Space-Based Atomic Partitions	Joan Grèbol-Tomàs
PB72	Spurious Oscillations In The Electronic Contributions To Nonlinear Optical Properties	Guillem Vila Siles
PB73	Simulation of experimental NMR signals from charge transfer complexes using novel quantum chemistry methods	Lu Liu
PB75	Parallel Implementation of Two-Photon Absorption Strengths Employing the Second-Order Algebraic Diagrammatic Construction Scheme for the Polarization Propagator	Friederike Schneider

Poster session 16. Materials2 - Antonio Márquez

Poster	Title	Speaker
PB76	Computational insights into the formation of tin halide perovskite nanostructures	Manuel Pérez escribano
PB77	Bond Length Isomerism in the Octasilacubane Si8(N(SiMe3)2)6	Christian Mück-Lichtenfeld
PB78	Exploring the Catalyst Function of Ionic Liquids in Polyethylene Terephthalate Glycolysis by Molecular Dynamics Simulations	Mohamed Nosir
PB79	Theoretical Study of the Mechanical Properties of PP-EPDM Materials	Mikel Irigoyen Urtasun
PB80	Computational characterization of the Persistent Organic Pollutants: adsorption, detection and permeability	Nicolás Ramos Berdullas
PB81	Modeling thermodynamics of an unexpected disordered copper-titanium telluride	J. Manuel Recio
PB82	Band structure, density of states, and charge transport properties of substituted Zn (II) and Si (IV) phthalocyanines	Gloria Cardenas-Jiron
PB83	Charting the thermoelectric performance of BiN combining DFT, Machine Learning and the BTE	Elena R. Remesal
PB84	Anharmonic effects in the lattice dynamics of BTBT	Guillermo Santamaría Fernández
PB85	First-Principles Anharmonic IR and Raman Spectra of Materials: Fermi Resonance in Dry Ice	Davide Mitoli