



2ona REUNIÓ DE QUÍMICA INORGÀNICA I ORGANOMETÀL·LICA de la SCQuímica



Programa Científic

| Dimecres, 5 de Febrer | | Dijous, 6 de Febrer | | Divendres, 7 de Febrer | |
|-----------------------|---|---------------------|--|------------------------|--|
| | | Sessió III | Moderador: Albert Figuerola Patrocinat per Inorg. Chem. | Sessió VII | Moderadora: Núria Aliaga-Alcalde Patrocinat per Adv. Catal. |
| | | 9:00-9:45 | Plenària 2 Eva Rentschler | 9:00-9:45 | Plenària 4 Alicia Forment |
| | | 9:45-10:00 | Contribució Oral 9 <i>Yulia Nelyubina</i> | 9:45-10:00 | Contribució Oral 22 <i>Mircea Dincă</i> |
| | | 10:00-10:15 | Contribució Oral 10 <i>Rosa Diego</i> | 10:00-10:15 | Contribució Oral 23 <i>Leví Arrieche-Hernández</i> |
| | | 10:15-10:30 | Contribució Oral 11 <i>Silvia Gómez-Coca</i> | 10:15-10:30 | Contribució Oral 24 <i>Pilar Fernández-Seriñán</i> |
| | | 10:30-11:10 | Flash 1 – 8 | 10:30-11:10 | Flash 20 – 26 + Joves SCQ |
| | | 11:10-11:35 | Pausa Cafè Sessió Pòsters | 11:10-11:35 | Pausa Cafè Sessió Pòsters |
| | | Sessió IV | Moderadora: Rosario Núñez | Sessió VIII | Moderadora: Mónica H. Pérez-Temprano Patrocinat per AstraZeneca |
| | | 11:35-11:50 | Contribució Oral 12 <i>Clara Viñas</i> | 11:35-11:50 | Contribució Oral 25 <i>Valentin Novikov</i> |
| | | 11:50-12:05 | Contribució Oral 13 <i>Andrea Álvarez-Núñez</i> | 11:50-12:05 | Contribució Oral 26 <i>Núria Aliaga-Alcalde</i> |
| | | 12:05-12:20 | Contribució Oral 14 <i>Araceli de Aquino</i> | 12:05-12:20 | Contribució Oral 27 <i>Jose Muñoz</i> |
| | | 12:20-12:45 | Flash 9 – 13 | 12:20-12:35 | Contribució Oral 28 <i>Roc Matheu</i> |
| | | 12:45-13:00 | Contribució Oral 15 <i>Arántzazu González-Campo</i> | 12:35-13:20 | Plenària 5 Cathleen Crudden |
| | | 13:00-13:15 | Contribució Oral 16 <i>Carles Fuertes-Espinosa</i> | | |
| | | 13:15-13:30 | Foto de grup | 13:20-13:40 | Cloenda i Premis |
| 14:00-15:30 | Inscripcions | 13:30-16:00 | Dinar | | |
| 15:30-15:45 | Benvinguda i Obertura | | | | |
| Sessió I | Moderador: Oscar Pàmies Patrocinat per AstraZeneca | Sessió V | Moderador: Miquel Costas Patrocinat per Organometal·lics | | |
| 15:45-16:30 | Plenària 1 Per-Ola Norrby | 16:00-16:45 | Plenària 3 Alicia Casitas | | |
| 16:30-16:45 | Contribució Oral 1 <i>Maria Besora</i> | 16:45-17:00 | Contribució Oral 17 <i>Yisong Wen</i> | | |
| 16:45-17:00 | Contribució Oral 2 <i>Albert Solé-Daura</i> | 17:00-17:30 | Flash 14 – 19 | | |
| 17:00-17:15 | Contribució Oral 3 <i>Filippo Scarchilli</i> | 17:30-18:00 | Pausa Cafè Sessió Pòsters | | |
| 17:15-17:30 | Contribució Oral 4 <i>Carla Alamillo Ferrer</i> | Sessió VI | Moderador: Xavi Ribas | | |
| Sessió II | Moderador: Carles Bo | 18:00-18:15 | Contribució Oral 18 <i>Arnald Grabulosa</i> | | |
| 17:30-17:45 | Contribució Oral 5 <i>Albert Poater</i> | 18:15-18:30 | Contribució Oral 19 <i>Mireia Pujol</i> | | |
| 17:45-18:00 | Contribució Oral 6 <i>Isabel Guerrero</i> | 18:30-18:45 | Contribució Oral 20 <i>Ricardo Castarlenas</i> | | |
| 18:00-18:15 | Contribució Oral 7 <i>Joaquín Soriano-López</i> | 18:45-19:00 | Contribució Oral 21 <i>Javier Ordóñez-Hernández</i> | | |
| 18:15-18:30 | Contribució Oral 8 <i>Bahareh Khezri</i> | | | | |
| 18:30-20:30 | Sopar de Benvinguda | 20:45 | Sopar de Gala <i>Hotel Imperial Tarraco</i> <i>Sala Forum</i> | | |

Taula de continguts

| Plenàries | | 10 |
|---------------------|---|----|
| PL1. | <i>Predicting reaction selectivity</i> Per-Ola Norrby – AstraZeneca, Suècia | 11 |
| PL2. | <i>Metallacrown complexes: Host-guest interaction paving the way for molecular magnets</i> Eva Rentschler – Johannes Gutenberg University Mainz, Alemanya | 12 |
| PL3. | <i>An organometallic perspective to first-row transition metal catalysis</i> Alicia Casitas – Philipps-Universität Marburg, Alemanya | 13 |
| PL4. | <i>Transition metal chalcogenides 2D materials: A playground for chemistry</i> Alicia Forment – Universitat de València, Espanya | 14 |
| PL5. | <i>The power of organometallics: From catalysts to self-assembled monolayers to atomically precise nanoclusters</i> Cathleen Crudden – Queen's University, Canadà | 15 |
| Contribucions Orals | | 16 |
| CO1. | <i>In depth study of the polyoxometalate catalyzed water oxidation: electrochemical, chemical and statistical approaches</i> Maria Besora – Universitat Rovira i Virgili, Espanya | 17 |
| CO2. | <i>Computational insights into photocatalytic CO₂ reduction by polyoxometalate-based complexes and materials</i> Albert Solé-Daura – Institut Català d'Investigació Química, Espanya | 18 |
| CO3. | <i>Highly selective C(sp³)-H bond oxygenation at remote methylenic sites enabled by polarity enhancement</i> Filippo Scarchilli – Universitat de Girona, Espanya | 19 |
| CO4. | <i>From reactants to products: the role of NMR in reaction progress analysis</i> Carla Alamillo Ferrer – Institut Català d'Investigació Química, Espanya | 20 |
| CO5. | <i>Late-stage functionalization of pharmaceuticals by C-C cross-coupling enabled by wingtip flexible N-heterocyclic carbenes</i> Albert Poater – Universitat de Girona, Espanya | 21 |
| CO6. | <i>Sustainable photoredox catalysis with metallabis(dicarbollides): From small alkenes to unsaturated fatty acids</i> Isabel Guerrero – Institut de Ciència de Materials de Barcelona, Espanya | 22 |
| CO7. | <i>Polyoxometalate-layered double hydroxide nanocomposites as water oxidation electrocatalysts</i> Joaquín Soriano-López – Universitat de València, Espanya | 23 |
| CO8. | <i>Synergistic composite materials for electrochemical CO₂ reduction and hydrogen generation</i> Bahareh Khezri – Universitat Rovira i Virgili, Espanya | 24 |
| CO9. | <i>In situ NMR search for switchable magnetic compounds</i> Yulia Nelyubina – A. N. Nesmeyanov Institute of Organoelement Compounds, Rússia | 25 |



2ona REUNIÓ DE QUÍMICA INORGÀNICA I ORGANOMETÀL·LICA de la



| | | |
|-------|--|----|
| CO10. | <i>Square-lattice to square-complex: Radical-pyrazine architectures</i> Rosa Diego – Universitat de Bordeaux, França | 26 |
| CO11. | <i>The encapsulation of ferrocenium in an organic hosts enhances spin relaxation</i> Silvia Gómez-Coca – Universitat de Barcelona, Espanya | 27 |
| CO12. | <i>Revolutionizing nanomedicine: how tiny amphiphilic molecules are transforming drug delivery and therapy</i> Clara Viñas – Institut de Ciència de Materials de Barcelona, Espanya | 28 |
| CO13. | <i>Exploring the intramolecular chemistry of iron(V)-oxo-carboxylato species</i> Andrea Álvarez-Núñez – Universitat de Girona, Espanya | 29 |
| CO14. | <i>Exploring anion-dependent photophysical properties of Ag(I) and Au(I) pillarplexes</i> Araceli de Aquino – Universitat de Barcelona, Espanya | 30 |
| CO15. | <i>Curminoid-based active surfaces towards the preparation of sensors</i> Arántzazu González-Campo – Institut de Ciència de Materials de Barcelona, Espanya | 31 |
| CO16. | <i>Light-driven molecular motors within confined spaces</i> Carles Fuertes-Espinosa – Universitat de Girona, Espanya | 32 |
| CO17. | <i>Cyclometallated iridium catalysts for the asymmetric hydrogenation of imines</i> Yisong Wen – Institut de Recerca Biomèdica de Barcelona, Espanya | 33 |
| CO18. | <i>Cyclometallated pyrenylphosphanes half-sandwich complexes: A promising new motif in antitumoral drug design</i> Arnald Grabulosa – Universitat de Barcelona, Espanya | 34 |
| CO19. | <i>Stereoselective control on Cu activation of β,β-diboryl acrylates for allylic coupling protocols with concomitant lactonization reactions</i> Mireia Pujol – Universitat Rovira i Virgili, Espanya | 35 |
| CO20. | <i>Ligand-controlled chemoselectivity between dimerization and (2+2+1) cyclootrimerization of alkynes catalyzed by Rh-NHC-BHetA architectures</i> Ricardo Castarlenas – Universidad de Zaragoza, Espanya | 36 |
| CO21. | <i>Biocompatible boron cluster-based photoluminescent dyes as effective antimicrobial photosensitizers</i> Javier Ordóñez-Hernández – Institut de Ciència de Materials de Barcelona, Espanya | 37 |
| CO22. | <i>Catalysis with metal-organic frameworks: Opportunities in commodity chemicals</i> Mircea Dincă – Massachusetts Institute of Technology, United States | 38 |
| CO23. | <i>Effect of the acid and metallic properties of Ni/H-zeolite catalysts on the obtention of biofuels from 5-hydroxymethylfurfural</i> Leví Arrieche-Hernández – Universitat Rovira i Virgili, Espanya | 39 |
| CO24. | <i>Clip-off chemistry as a novel approach to obtain metal-organic nanosheets</i> Pilar Fernández-Seriñán – Universitat Autònoma de Barcelona, Espanya | 40 |
| CO25. | <i>Make the design molecular again: metal cage complexes for spintronic devices</i> Valentin Novikov – Universitat de Barcelona, Espanya | 41 |
| CO26. | <i>Interplay of curcuminoid design and deposition methods for their electronic applications</i> Núria Aliaga-Alcalde – Institut de Ciència de Materials de Barcelona, Espanya | 42 |

| | | |
|----------------------------|--|-----------|
| CO27. | <i>Unveiling the chemical reactivity of Ge-based 2D materials with thiolated molecules: Functionalization, passivation and (bio)applications</i> | 43 |
| | Jose Muñoz – Universitat Autònoma de Barcelona, Espanya | |
| CO28. | <i>Redox-active and -inactive molecules inside expanded halide perovskite analogs can behave as charge reservoirs</i> | 44 |
| | Roc Matheu – Universitat de Barcelona, Espanya | |
| Contribucions Flash | | 45 |
| CF1. | <i>Schiff bases as platform for synthesising molecular magnets</i> | 46 |
| | Ernesto Costa-Villén | |
| CF2. | <i>Effect of 2,2'-bipyridine ligand on ruthenium nanoparticles for hydrogen evolution catalysis</i> | 47 |
| | Álvaro Lozano-Roche | |
| CF3. | <i>Designing switchable materials: The role of supramolecular interactions in Fe(II) spin-crossover</i> | 48 |
| | Raúl Díaz-Torres | |
| CF4. | <i>Synthesis of metal-organic cages via orthogonal bond cleavage in 3D metal-organic frameworks</i> | 49 |
| | Sara Ruiz-Relaño | |
| CF5. | <i>Supramolecular mask regio-converter: Orthogonal Diels-Alder C₇₀ bis-adducts by mask-mediated regioselective synthesis</i> | 50 |
| | Tània Pèlachs i Monell | |
| CF6. | <i>Estudi computacional del moviment d'un guest planar dins d'un metal-lorectangle</i> | 51 |
| | Mercè Alemany-Chavarria | |
| CF7. | <i>Un enfocament microcinètic híbrid per connectar teoria i experiments en l'oxidació de l'aigua</i> | 52 |
| | Mireia Segado Centellas | |
| CF8. | <i>Remote 1,4-carbon-to-carbon boryl migration: From a mechanistic challenge to a valuable synthetic application of bicycles</i> | 53 |
| | Paula Dominguez-Molano | |
| CF9. | <i>Ni nanocatalysts in an inorganic matrix for OER at pH 7</i> | 54 |
| | Aureliano Macili | |
| CF10. | <i>Predicció de l'especiació aquosa de heteropolioxometalats: el fosfomolibdat i l'arsenomolibdat</i> | 55 |
| | Jordi Buils | |
| CF11. | <i>Integrating molecular spin qubits in multidimensional systems</i> | 56 |
| | Joan Torrent | |
| CF12. | <i>Ru-based heterogeneous catalytic systems for organic photoactivated oxidations</i> | 57 |
| | Rabab Maqsood | |
| CF13. | <i>Molecular anodes for electrocatalytic water oxidation based on self assembled bilayers driven by electron transfer mediators</i> | 58 |
| | Paula Tris-Marzo | |
| CF14. | <i>Towards efficient asymmetric hydrogenation of tetrasubstituted enones: New catalyst design and mechanistic insights</i> | 59 |
| | Jorge Faiges | |

| | | |
|----------------|---|-----------|
| CF15. | <i>Cu-catalyzed asymmetric synthesis of γ-amino alcohols featuring tertiary carbon stereocenters</i> | 60 |
| | Alejandro Delgado | |
| CF16. | <i>Asymmetric γ-C-H lactonization as a new approach for the synthesis of quaternary chiral malonates</i> | 61 |
| | Nikolaos Siakavaras | |
| CF17. | <i>Rh-catalyzed single-carbon insertion of 1,3-dienes</i> | 62 |
| | Norman Díaz | |
| CF18. | <i>Cu-catalyzed enantioselective borylative desymmetrization of 1-vinyl cyclobutanols and axial-to-point chirality transfer in a diastereoconvergent/stereoretentive allylation scenery</i> | 63 |
| | Nerea Irigorri | |
| CF19. | <i>Dearomatizative oxidation of arenes</i> | 64 |
| | Najoua Choukairi Afaïal | |
| CF20. | <i>Sulfanilic acid-capped Ru-NPs for enhanced HER activity in neutral media</i> | 65 |
| | Matilda Kraft | |
| CF21. | <i>Synthesis and characterization of well-ordered mesoporous carbons from almond shells as the biomass source</i> | 66 |
| | Jennifer Lozano Castro | |
| CF22. | <i>La química supramolecular i l'efecte plantilla com a eines estratègiques per a la construcció d'arquitectures heterolèptiques dinuclears de Ni(II)</i> | 67 |
| | Jordi Martínez Morató | |
| CF23. | <i>A versatile synthesis method of OD-metal nanoparticle@2D-germanane nanoarchitectonics for energy conversion and biosensor implementations</i> | 68 |
| | Yiming Lei | |
| CF24. | <i>Slow magnetic relaxation in Ag(II) macrocyclic systems</i> | 69 |
| | Joan Serra | |
| CF25. | <i>Computational evaluation of the role of the overcharge protector in electrochemical cross-electrophile coupling</i> | 70 |
| | Marina Díaz-Ruiz | |
| CF26. | <i>Pivotal synthesis of tetrasubstituted epoxides from ketones and α-halo B/Si ylides</i> | 71 |
| | Luis Tarifa | |
| Pòsters | | 72 |
| P1. | <i>Advanced metallocarborane photocatalysts for efficient removal of organic compounds in surface and wastewater effluent</i> | 73 |
| | Nabila Mimouni | |
| P2. | <i>Synthesis of new aminophosphine/phosphoramidite-pyridine ligands for Ir-catalyzed asymmetric hydrogenation of olefins</i> | 74 |
| | José Antonio García-Alcázar | |
| P3. | <i>The development of readily accessible phosphinite/phosphite-triazole ligands for Ir-catalyzed asymmetric hydrogenation of alkenes</i> | 75 |
| | Zahid Hussain | |

| | | |
|------|---|----|
| P4. | <i>Pd-catalyzed allylic substitution using nucleophilic amines: Access to functionalized mono- and bis-N-allyl synthons</i> Fengyun Gao | 76 |
| P5. | <i>Synthesis of 2-oxabicyclic [2.2.1] heptanes using a binary Al(III) complex/halide catalyst</i> Chenyang Chang | 77 |
| P6. | <i>Synthesis of luminescent curved nanographene-like compounds via the Scholl reaction</i> Judith Sala | 78 |
| P7. | <i>A versatile, readily available and bench stable iron catalyst active in carbene transfer reactions</i> David Capellán | 79 |
| P8. | <i>Synthesis and characterization of new Mn complexes and their application in the asymmetric directed oxidation of non-activated C-H bonds</i> Eric Aparicio | 80 |
| P9. | <i>Organometallic complexes of Au(I) with azobenzene derivative ligands: Study of the photodynamic process</i> Ot Raich Panisello | 81 |
| P10. | <i>Cu-catalyzed Boron-Wittig reactions of carbonylic compounds</i> Carmen María Arenas | 82 |
| P11. | <i>Supramolecularly directed enantioselective γ-lactonization of carboxylic acids using bioinspired manganese catalysts</i> Christos Christou | 83 |
| P12. | <i>Towards the quantum properties' manipulation of metallohelicate-based host-guest supramolecular assemblies</i> Konstantinos Sotirakopoulos | 84 |
| P13. | <i>Nous complexos polinuclears de lantànids per a aplicacions de computació quàntica i conversió ascendent de fotons</i> José Serrano-Guarinos | 85 |
| P14. | <i>Exploring copper β-diketimate complexes for heterogeneous ammonia oxidation on graphitic surfaces via CH-π and π-π interactions</i> Josep Antoni Gutiérrez-Orgaz | 86 |
| P15. | <i>Bimetallic alloy nanoparticles immobilized over TiO₂ nanostructures for enhanced CO₂ photoreduction</i> Yaroslav Hryhoryev | 87 |
| P16. | <i>Encapsulation of fullerenes and stabilization of their radical anions for characterization and functionalization via supramolecular mask strategies</i> Piyush Piyush | 88 |
| P17. | <i>Exploring mechanistic insights of Cp*CoIII-catalyzed C-H functionalizations with organometallic nucleophiles</i> Sergio Barranco | 89 |
| P18. | <i>Computational study of Rh(II)/Pd(0) dual catalysis in the synthesis of 2,2-disubstituted tetrahydroquinolines</i> Edmond Apaloo-Messan | 90 |
| P19. | <i>Photoinduced water oxidation using organic photosensitizers and a copper (II) catalyst</i> Elena Bassan | 91 |



| | | |
|-------------|--|----|
| P20. | <i>Study of the spin dynamics of a new family of Schiff base heterometallic complexes containing 3d-4f metals</i> Sergio Caballero | 92 |
|-------------|--|----|