



1a REUNIÓ DE QUÍMICA INORGÀNICA I ORGANOMETÀL·LICA de la SCQ



Scientific Program

| Thursday, February 2 | | Friday, February 3 | |
|----------------------|--|---------------------|---|
| 9:00-9:30 | Registrations | | |
| 9:30-9:45 | Welcome. Prof. G. Aromí | SESSION V | Chair Laura Rodríguez Sponsored by Adv. Catal. Elsevier. |
| | Opening. Prof. G. Ujaque | 9:20-10:00 | Plenary 3. Corine Mathonière |
| SESSION I | Chair Miquel A. Pericàs Sponsored by AstraZeneca | 10:00-10:20 | Oral Communication 15. <i>J. Puigmartí-Luis</i> |
| 9:50-10:30 | Plenary 1. Ruben Martin | 10:20-10:40 | Oral Communication 16. <i>R. Núñez</i> |
| 10:30-10:50 | Oral Communication 1. <i>S. Rafael</i> | 10:40-11:00 | Oral Communication 17. <i>M. Martínez</i> |
| 10:50-11:10 | Oral Communication 2. <i>M. Biosca</i> | 11:00-11:30 | Coffee Break-Poster Session |
| 11:10-11:40 | Coffee Break-Poster Session | SESSION VI | Chair Daniel Maspoch |
| SESSION II | Chair E. Carolina Sañudo Sponsored by AstraZeneca | 11:30-11:50 | Oral Communication 18. <i>A. Figuerola</i> |
| 11:40-12:00 | Oral Communication 3. <i>X. Sala</i> | 11:50-12:10 | Oral Communication 19. <i>L. Capdevila</i> |
| 12:00-12:20 | Oral Communication 4. <i>L. Francàs</i> | 12:10-12:30 | Oral Communication 20. <i>E. C. Sañudo</i> |
| 12:20-12:40 | Oral Communication 5. <i>I. Fort-Grandas</i> | 12:30-12:50 | Oral Communication 21. <i>A. Carné-Sánchez</i> |
| 12:40-13:00 | Oral Communication 6. <i>A. de Aquino</i> | 12:50-13:10 | Oral Communication 22. <i>A. Cortés-Martínez</i> |
| 13:00-13:20 | Oral Communication 7. <i>R. Matheu</i> | 13:10-13:15 | Presentation of the Young Section of the SCQ |
| 13:20-15:30 | Lunch – Poster Session | 13:15-13:20 | Group Picture |
| | | 13:20-15:30 | Lunch – Poster Session |
| SESSION III | Chair Arjan. W. Kleij Sponsored by Organometallics and Inorg. Chem. | SESSION VII | Chair Xavier Sala Sponsored by Adv. Catal. Elsevier. |
| 15:30-16:10 | Plenary 2. Eva Hevia | 15:30-16:10 | Plenary 4. Guillermo Minguez |
| 16:10-16:30 | Oral Communication 8. <i>M. Sethuraman</i> | 16:10-16:30 | Oral Communication 23. <i>R. Diego</i> |
| 16:30-16:50 | Oral Communication 9. <i>M. Galeotti</i> | 16:30-16:50 | Oral Communication 24. <i>S. Ruiz-Relaño</i> |
| 16:50-17:20 | Coffee Break-Poster Session | 16:50-17:20 | Coffee Break-Poster Session |
| SESSION IV | Chair Anna Company Sponsored by Organometallics and Inorg. Chem. | SESSION VIII | Chair Montserrat Ferrer |
| 17:20-17:40 | Oral Communication 10. <i>C. Casadevall</i> | 17:20-17:40 | Oral Communication 25. <i>E. Petrus</i> |
| 17:40-18:00 | Oral Communication 11. <i>J. Margalef</i> | 17:40-18:00 | Oral Communication 26. <i>N. Pagès-Vilà</i> |
| 18:00-18:20 | Oral Communication 12. <i>S. Barranco</i> | 18:00-18:20 | Oral Communication 27. <i>P. Font</i> |
| 18:20-18:40 | Oral Communication 13. <i>A. Garcia-Roca</i> | 18:20-18:40 | Closing Ceremony. Prof. M. Diéguez |
| 18:40-19:00 | Oral Communication 14. <i>J. Eusamio</i> | | |
| 20:30 | Conference Dinner | | |



1a REUNIÓ DE QUÍMICA INORGÀNICA I ORGANOMETÀL·LICA de la SCQ



Thursday, February 2

| | |
|-------------------|---|
| 9:00-9:30 | Registrations |
| 9:30-9:45 | Welcome. Prof. Guillem Aromí |
| | Opening. Prof. Gregori Ujaque |
| SESSION I | Chair Miquel A. Pericàs Sponsored by AstraZeneca |
| 9:50-10:30 | Plenary 1. Ruben Martin . <i>Taming multifaceted nickel catalysts: an academic fascination</i> |
| 10:30-10:50 | Oral Communication 1. Sergi Rafael . <i>Synthesis and application of internal ynamides in the Pauson-Khand reaction</i> |
| 10:50-11:10 | Oral Communication 2. Maria Biosca . <i>Readily available tailor-made Ir-catalysts for the enantioselective reduction of challenging substrates</i> |
| 11:10-11:40 | Coffee Break-Poster Session |
| SESSION II | Chair E. Carolina Sañudo Sponsored by AstraZeneca |
| 11:40-12:00 | Oral Communication 3. Xavier Sala . <i>Surface-functionalized nanomaterials for the production of solar fuels</i> |
| 12:00-12:20 | Oral Communication 4. Laia Francàs . <i>Deciphering the key factors for the good performance of different Ni/NiOOH electrocatalysts</i> |
| 12:20-12:40 | Oral Communication 5. Ignasi Fort-Grandas . <i>Study of conductive MOFs based on triphenylene derivatives for chemiresistive greenhouse gas sensors</i> |
| 12:40-13:00 | Oral Communication 6. Araceli de Aquino . <i>Compostos supramoleculares d'or(I) amb propietats fosforescents</i> |
| 13:00-13:20 | Oral Communication 7. Roc Matheu . <i>Charge reservoirs in an expanded halide perovskite analog: enhancing high-pressure conductivity through redox-active molecules</i> |
| 13:20-15:30 | Lunch – Poster Session |



1a REUNIÓ DE QUÍMICA INORGÀNICA I ORGANOMETÀL·LICA de la SCQ



| | |
|--------------------|---|
| SESSION III | Chair Arjan. W. Kleij Sponsored by Organometallics and Inorg. Chem. |
| 15:30-16:10 | Plenary 2. Eva Hevia . <i>Tailoring organosodium reagents for new synthetic and catalytic applications</i> |
| 16:10-16:30 | Oral Communication 8. Muthuramalingam Sethuraman . <i>Oxidative desymmetrization of cyclic amides via enantioselective C-H bond oxidation using bioinspired manganese catalysts</i> |
| 16:30-16:50 | Oral Communication 9. Marco Galeotti . <i>Manganese-catalyzed C-H bond oxidation of cyclopropane containing hydrocarbons</i> |
| 16:50-17:20 | Coffee Break-Poster Session |
| SESSION IV | Chair Anna Company Sponsored by Organometallics and Inorg. Chem. |
| 17:20-17:40 | Oral Communication 10. Carla Casadevall . <i>Carbon-based materials for solar-driven catalysis</i> |
| 17:40-18:00 | Oral Communication 11. Jèssica Margalef . <i>Reversed regioselectivity in the Rh-hydroformylation of styrene</i> |
| 18:00-18:20 | Oral Communication 12. Sergio Barranco . <i>Merging Cp*Co catalysis and statistical analysis for interrogating deuterium source selection in directed hydrogen isotope exchange</i> |
| 18:20-18:40 | Oral Communication 13. Alèria Garcia-Roca . <i>A comprehensive mechanistic scenario for the Cu-mediated asymmetric propargylic sulfonylation forging tertiary carbon stereocenters</i> |
| 18:40-19:00 | Oral Communication 14. Javier Eusamio . <i>P-Stereogenic non-symmetric diphosphanes with a methylene bridge: coordination chemistry to late transition metals</i> |
| 20:30 | Conference Dinner |



1a REUNIÓ DE QUÍMICA INORGÀNICA I ORGANOMETÀL·LICA de la SCQ



Friday, February 3

| | |
|-------------|--|
| SESSION V | Chair Laura Rodríguez Sponsored by Adv. Catal. Elsevier. |
| 9:20-10:00 | Plenary 3. Corine Mathonière. <i>Switchable cyanometallate compounds : Metal-to-metal charge transfer or spin crossover?</i> |
| 10:00-10:20 | Oral Communication 15. Josep Puigmartí-Luis. <i>Microfluidic technologies as an advanced tool for chemistry and materials synthesis</i> |
| 10:20-10:40 | Oral Communication 16. Rosario Núñez. <i>Inorganic boron clusters as unique entities to trigger and modulate molecule and material properties</i> |
| 10:40-11:00 | Oral Communication 17. Manuel Martínez. <i>Building molecular mixed-valence cyanido-bridged Coll/Fell redox active complexes: from dinuclear to cubic species</i> |
| 11:00-11:30 | Coffee Break-Poster Session |
| SESSION VI | Chair Daniel MasPOCH |
| 11:30-11:50 | Oral Communication 18. Albert Figuerola. <i>Synthesis and applications of group 11-based ternary Semiconductor nanocrystals with tunable morphology and composition</i> |
| 11:50-12:10 | Oral Communication 19. Lorena Capdevila. <i>Synthesis of curved perylene-based nanographenes</i> |
| 12:10-12:30 | Oral Communication 20. E. Carolina Sañudo. <i>Devices for quantum computing: towards a measurement of on-surface qubit phase memory time</i> |
| 12:30-12:50 | Oral Communication 21. Arnau Carné-Sánchez. <i>Reactivitat i assemblatge de poliedres metal-orgànics</i> |
| 12:50-13:10 | Oral Communication 22. Alba Cortés-Martínez. <i>Síntesi de materials oligomèrics porosos</i> |
| 13:10-13:15 | Presentation of the Young Section of the SCQ |
| 13:15-13:20 | Group Picture |
| 13:20-15:30 | Lunch – Poster Session |



1a REUNIÓ DE QUÍMICA INORGÀNICA I ORGANOMETÀL·LICA de la SCQ



| | |
|---------------------|--|
| SESSION VII | Chair Xavier Sala Sponsored by Adv. Catal. Elsevier. |
| 15:30-16:10 | Plenary 4. Guillermo Mínguez . <i>Porous materials with electroactive building blocks</i> |
| 16:10-16:30 | Oral Communication 23. Rosa Diego . <i>Quantum fluctuations in single molecule magnets on magnetic substrates</i> |
| 16:30-16:50 | Oral Communication 24. Sara Ruiz-Relaño . <i>Síntesi de noves estructures metal·loorgàniques mitjançant la química de "Clip-Off"</i> |
| 16:50-17:20 | Coffee Break-Poster Session |
| SESSION VIII | Chair Montserrat Ferrer |
| 17:20-17:40 | Oral Communication 25. Enric Petrus . <i>Predint l'especiació en dissolució aquosa i els mecanismes d'auto-assemblatge dels òxids metàl·lics moleculars de Mo, W, V, Nb i Ta</i> |
| 17:40-18:00 | Oral Communication 26. Neus Pagès-Vilà . <i>Proton triggered chemoselective halogenation of aliphatic C-H bonds with nonheme Fe(IV)-oxo complexes. An alternative model for nonheme halogenases</i> |
| 18:00-18:20 | Oral Communication 27. Pau Font . <i>Hemilabile MIC^N ligands allow oxidant-free Au(I)/Au(III) arylation-lactonization of γ-alkenoic acids</i> |
| 18:20-18:40 | Closing Ceremony. Prof. Montserrat Diéguez |

Posters

| | |
|-----------|--|
| Poster 1 | Ànnia Tubau. $[Dy_2(\mu-2,6-2FBz)_4(NO_3)_4]^{2-}$ and $[Dy_2(\mu-2,6-2FBz)_4(2,6-2FBz)_4]^{2-}$: Two anhydrous different structural motifs depending on the solvent |
| Poster 2 | Yuzelfy Mendoza-Gamero. Triphenylene derivative MOFs for greenhouse gas sensing and green catalysis |
| Poster 3 | Pol de la Cruz-Sánchez. Enhancing Pd-catalyzed asymmetric allylic substitution reactions with improved catalysts for the construction of chiral C-C and C-X bonds |
| Poster 4 | Jorge Faiges. DFT guided ligand design for iridium catalyzed asymmetric hydrogenation. Filling the gap by in silico optimization |
| Poster 5 | María Dolores Fernández-Martínez. New supported phosphine-stabilized palladium nanocatalysts for the hydrogenation of CO ₂ into formate |
| Poster 6 | Jie Pan. Propane dehydrogenation over small platinum clusters supported on g-C ₃ N ₄ |
| Poster 7 | Álvaro Lozano-Roche. Is size all that matters? A discussion on the fine-tuning of metallic nanoparticles |
| Poster 8 | Daniel Tarr. A new Ir-P,N catalyst design to solve the asymmetric hydrogenation of challenging alkenes |
| Poster 9 | Qian Zeng. Stereoselective multi-component allylic alkylation enabled by dual photoredox/Ni catalysis |
| Poster 10 | Khalid Azmani. Understanding polyoxometalates as water oxidation catalysts through iron vs. cobalt reactivity |
| Poster 11 | Montserrat Ferrer. Cianuro complexos de Fe(II) amb grups azo solubles en aigua: estudi mecanístic de la seva isomerització tèrmica cis-trans |
| Poster 12 | Manuel Martínez. Kinetic-mechanistic studies on the lability of Cu(II)-carbon bonds: homo- or heterolysis? |
| Poster 13 | Yisong Wen. Cyclometallated iridium catalysts for the asymmetric hydrogenation of imines |
| Poster 14 | Marina Bellido. Three-component Suzuki-Miyaura/allylic substitution: a regioselective approach to 2-aryl allyl sulfones |
| Poster 15 | Sara López-Resano. Mechanistic insights into the oxidation of Cp*Co(III) species with F ⁺ oxidants |
| Poster 16 | Aureliano Macili. Tuning nanoparticles for artificial photosynthesis applications |
| Poster 17 | Laura Hernández-López. Switchable MOP solubility through surface chemistry: engineering molecular self-sorting systems |
| Poster 18 | Akim Khabotov-Bakishev. Polimerització covalent de caixes moleculars poroses: síntesi, funcionalització i aplicacions |

| | |
|-----------|--|
| Poster 19 | Leoni Alejandra Barrios. <i>L'efecte plantilla de l'anió SiF_6^{2-} i els ponts d'hidrogen: L'aliança perfecta per aconseguir la formació exclusiva de nous sistemes de coordinació heterolèptics</i> |
| Poster 20 | Manuel Imperato. <i>Synthesis of Ni(II) helicates for the chemical tuning of spin clock transitions</i> |
| Poster 21 | Jose Muñoz. <i>Design of functional inorganic 2D materials via molecular engineering</i> |
| Poster 22 | David Aguilà. <i>Disseny de compostos dinuclears de lantànid per portes lògiques quàntiques</i> |
| Poster 23 | Diamantoula Maniaki. <i>Highly selective heterometallic $[\text{LnLn}'\text{Ln}]$ molecules as 3-qubit quantum gates</i> |
| Poster 24 | Heting Hou. <i>Light-driven hydrogen evolution using Ni, Cu and Pt nanoparticles supported on carbon nitride and covalent triazine-frameworks</i> |
| Poster 25 | Adriana Silvestre-Llora. <i>Millora dels temps de relaxació de imants unimoleculars</i> |
| Poster 26 | Najoua Choukairi Afailal. <i>Dearomatizative syn-dihydroxylation of arenes</i> |
| Poster 27 | Andrea Palone. <i>C-H Bonds as functional groups. simultaneous generation of multiple stereocenters by enantioselective hydroxylation at unactivated tertiary C-H bonds</i> |
| Poster 28 | Adrià Juvanteny. <i>Synthesis and reactivity of organometallic nickel complexes relevant in carbon-carbon and carbon-heteroatom bond formation reactions</i> |
| Poster 29 | Andrea Álvarez-Núñez. <i>Exploring the intramolecular chemistry of iron(V)-oxo-carboxylato species</i> |
| Poster 30 | David Capellán. <i>Carbene transfer reactions catalyzed by an iron/lithium dual system</i> |
| Poster 31 | Judith Sala. <i>Development of a new protocol towards the synthesis of nanographene-like compounds via aromatic homologation catalysis</i> |
| Poster 32 | Tània Pèlachs. <i>Orthogonal regioselective bis-functionalization of C_{60} by Diels-Alder reaction via avant-garde supramolecular mask strategy</i> |
| Poster 33 | Siu-Chung Chan. <i>Biologically inspired C-H hydroxylation catalysis with metallocavitand</i> |
| Poster 34 | Valentina Iannace. <i>Regioselective bis-functionalization of fullerene C_{70} via supramolecular masks</i> |
| Poster 35 | Syrine Affes. <i>Molecular and hybrid materials based on metallocarboranes</i> |
| Poster 36 | Angie Carlyne Rueda. <i>Preparation of carbons with different morphologies from xylose obtained from almond shells: carbon microspheres and ordered mesoporous carbons</i> |
| Poster 37 | Anna Casadó. <i>Catalitzadors de Ni suportats en carbons mesoporosos ordenats, obtinguts a partir de lignina procedent de biomassa, per a la hidrodesoxigenació de guaiacol</i> |