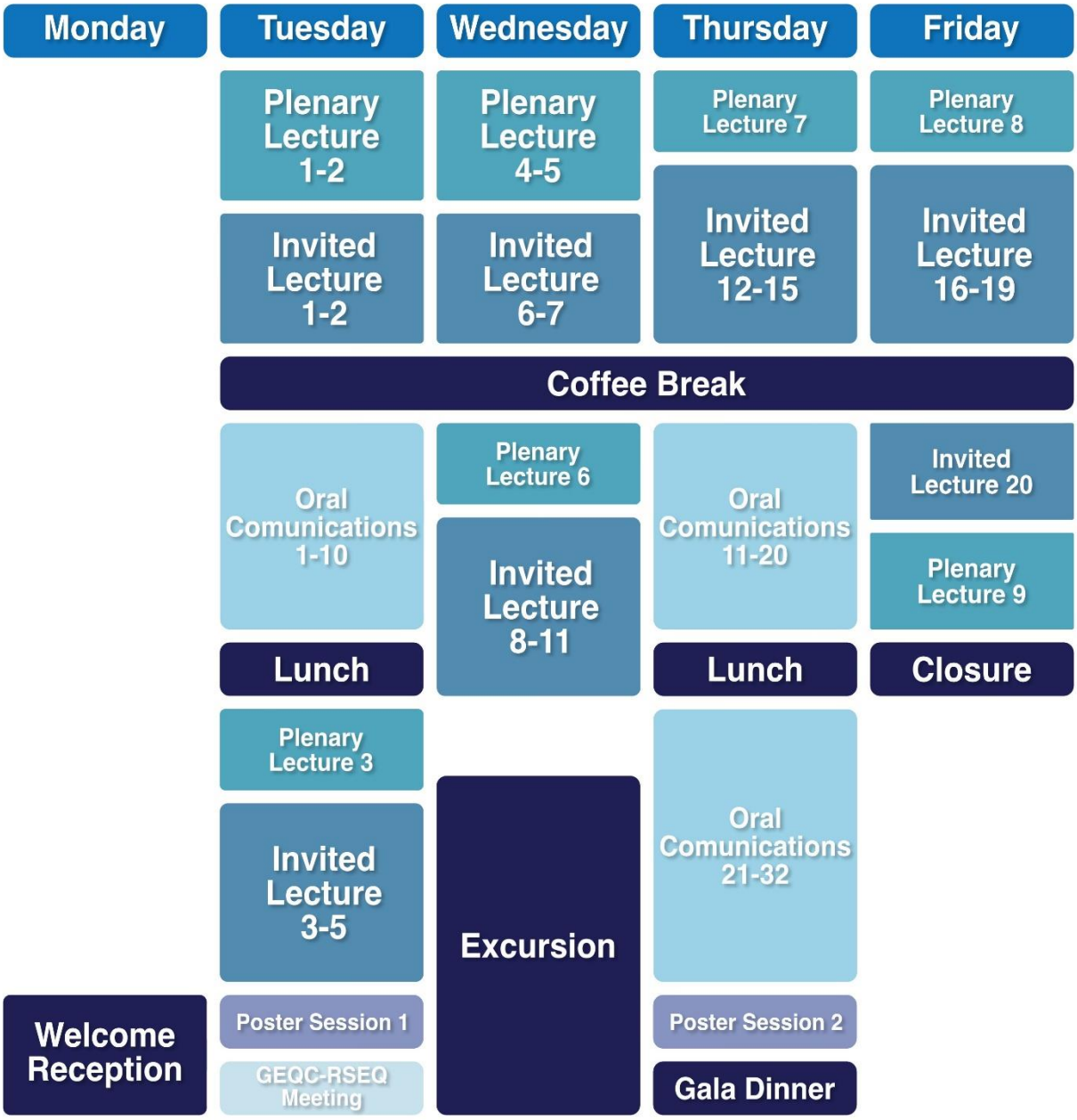
Electronic Structure Principles and Applications

and biannual Meeting of the RSEQ Group in Chemistry & Computation

June 3rd – 7th, 2024

Tarragona (Spain)



Monday, June 3:

18:30h: WELCOME RECEPTION

Tuesday, June 4:

SESSION 1:

- **9:00 - 9:45h:** PL1 - Silvia Osuna (Univ. de Girona, Spain): *Catalysis in confined spaces: insights from enzymatic to synthetic catalysts*
- **9:45 - 10:30h:** PL2 - Jochen Autschbach (Univ. at Buffalo, USA): *Chemical bonding and Molecular Properties*
- **10:30 - 10:50h:** IL1 - Marcella Iannuzzi (Univ. Zürich, Switzerland): *Probing Dynamics at Different Time Scales: an Investigation of Electron and Nuclei Behavior Through Density Functional Theory*
- **10:50 - 11:10h:** IL2 - Giovanni Li Manni (Max Planck Stuttgart, Germany): *Predicting Magnetic Interactions in Polynuclear Transition Metal Clusters via Quantum Anamorphosis*

11:10 - 11:40h: COFFE BREAK

SESSION 2a

- **11:40 - 12:00h:** OC1 - Enric Petrus (Swiss Federal Institute of Aquatic Science and Technology): *An Open-Source Methodology for Predicting the Aqueous Spectation: from Polyoxometalates to Environmental Chemistry*
- **12:00 - 12:20h:** OC2 - Miguel Gallegos (University of Oviedo): *Explainable Chemical AI (XCAI): beyond accurate predictions*
- **12:20- 12:40h:** OC3 - Lucia Morán-González (University of Oslo, Norway): *Seeking promising bifunctional catalysts for CO2 hydrogenation using active learning*
- **12:40 - 13:00h:** OC4 - Juan V. Alegre-Requena (CSIC - Universidad de Zaragoza): *Automated computational chemistry and machine learning workflows in chemistry*
- **13:00 - 13:20h:** OC5 - Johannes Gierschner (IMDEA Nanoscience, Madrid): *Rational Design of Color-Pure Blue All-Organic Emitters*

SESSION 2b

- **11:40 - 12:00h:** OC6 - Elisa Jimenez (Euskal Herriko Unibertsitatea (UPV/EHU), Donostia): *An exotic way for oxygen to dope graphene*

- **12:00 - 12:20h:** OC7 - Laura Abella (Universitat Rovira i Virgili, Tarragona): *Reactivity on Endohedral Metallofullerenes*
- **12:20- 12:40h:** OC8 - Silvia Gómez-Coca (University of Barcelona): *Magnetic Anisotropy, Magnetosructural Correlations and Spin-Phonon Coupling in Single-Molecule Magnets*
- **12:40 - 13:00h:** OC9 - Freiia De Vleeschouwer (Vrije Universiteit Brussel, Belgium): *Chemical space exploration towards novel and redox-active quinones for redox and flow batteries*
- **13:00 - 13:20h:** OC10 - Jean-Didier Maréchal (Universitat Autònoma de Barcelona): *A Methodological Framework to Study the Recruitment of Metals by Proteins*

13:20 - 15:30h: LUNCH

SESSION 3

- **15:30 - 16:15h:** PL3 - Fernanda Duarte (Univ. of Oxford, UK): *Computational Modelling of Supramolecular Metallo-organic Cages: Challenges and Opportunities*
- **16:15 - 16:35h:** IL3 - Albert Rimola (Univ. Autonoma de Barcelona, Spain): *Quantum Chemistry on Interstellar Grains*
- **16:35 - 16:55h:** IL4 - Cristina Trujillo (Univ. of Manchester, UK): *Computational Insights into Halogen-Bond-Based Organocatalysis*
- **16:55 - 17:15h:** IL5 - Israel Fernández (Complutense de Madrid, Spain): *The Pauli Repulsion Lowering Concept in Catalysis*

POSTER SESSION 1

GEQC-RSEQ Meeting

Wednesday, June 5:

SESSION 4:

- **9:00 - 9:45h:** PL4 - Sofia Calero (Eindhoven Univ., Netherlands): *Inventing materials to meet today's energy and environmental challenges*
- **9:45 - 10:30h:** PL5 - Stefan Grimme (Univ. Bonn, Germany): *GP3-xTB: DFT accuracy at tight-binding speed*

- **10:30 - 10:50h:** IL6 - Pablo García (Univ. de Cantabria, Spain): *Application of second-principles calculations to the simulation of optical and transport properties in solids*
- **10:50 - 11:10h:** IL7 - Sonsoles Martín-Santamaría (CIB-CSIC Madrid, Spain): *Molecular mechanisms of the innate immunity receptors through the computational glass*

11:10 - 11:40h: COFFE BREAK

SESSION 5

- **11:40 - 12:25h:** PL6 - Marco Eckhoff (ETH Zürich, Switzerland): *Lifelong machine learning potentials*
- **12:25- 12:45h:** IL8 - Carine Michel (ENS Lyon, France): *Modelling a Realistic Surface State of Metallic Supported Catalysts Working in Aqueous Phase Environment*
- **12:45 - 13:05h:** IL9 - Xabier López (Univ. del Pais Vasco, Spain): *Relevance of the conformational ensemble of selected intrinsically disordered peptides revealed by classical molecular dynamics simulations.*
- **13:05 - 13:25h:** IL10 - Marcos Mandado (Univ. de Vigo, Spain): *Combining CMD simulations with QM/MM-EDA to investigate intermolecular interactions in biological systems at finite temperatures*
- **13:25 - 13:45h:** IL11 - Carmen Jiménez Calzado (Univ. de Sevilla, Spain): *Spin-crossover molecules interacting with surfaces: a theoretical approach*

EXCURSION

Thursday, June 6:

SESSION 6:

- **9:00 - 9:45h:** PL7 - Anna Krylov (Univ. Southern California, USA): *Quantum chemistry of core-level states*
- **9:45 - 10:05h:** IL12 - Miquel Huix-Rotllant (Univ. Aix-Marseille, France): *Photoinduced intersystem crossing: a quantum dynamics perspective*
- **10:05 - 10:25h:** IL13 - Vera Krewald (TU Darmstadt, Germany): *Ab initio quantification of the nuclear dimensions for electron transfer*
- **10:25 - 10:45h:** IL14 - Stanislav Avdoshenko (Leibniz Institute, Germany): *Spins in cages: theoretical insights into molecular magnetism of endohedral*

metallofullerenes, quantification of FV-magnetism and models design for periodic systems

- **10:45 - 11:05h:** IL15 - Stella Stopkowicz (Saarland Univ., Germany): *Assignment of spectra and electronic structure of atoms and molecules in strong magnetic fields*

11:05 - 11:40h: COFFE BREAK

SESSION 7a

- **11:40 - 12:00h:** OC11 - Jen-Shiang K. Yu (National Yang Ming Chiao Tung University, Taiwan): *Characterization of enol ether intermediates in the intramolecular Stetter reactions by density functional theory and kinetic simulations*
- **12:00 - 12:20h:** OC12 - Ruben Laplaza (École Polytechnique Fédérale de Lausanne, Switzerland): *Nacigating homogeneous catalyst landscapes*
- **12:20- 12:40h:** OC13 - Kyoung Koo Baeck (Gangneung-Wonju National University, South Korea): *Microscopic dynamics of proton-coupled electron-transfer process in the case of bidirectional PCET from the charge-transferred excited state of FHCl*
- **12:40 - 13:00h:** OC14 - Milena Petkovic (University of Belgrade, Serbia): *Hydroboration of imines: Mechanistic insight provided by Relative Energy Gradient analysis*
- **13:00 - 13:20h:** OC15 - Hassan Rabaa (Ibn Tofail University, Morocco): *Theoretical study of unusual bonding of interaction of closed shell d10-d10 in a series of Heterobimetallic Complexes of Monovalent Group 10 and 11 Metal Centers*

SESSION 7b

- **11:40 - 12:00h:** OC16 - Miguel Recio (University of Barcelona): *Tuning electronic levels in photoactive hydroxylated titania nanosystems: combining the ligand dipole effect and quantum confinement*
- **12:00 - 12:20h:** OC17 - Luis Manuel Frutos (University of Alcala): *Computational mechano-photochemistry*
- **12:20- 12:40h:** OC18 - Marta Erminia Alberto (University of Calabria, Italy): *Recent strategies to afford hypoxia enhancing PDT*

- **12:40 - 13:00h:** OC19 - Lucía López-Pacios (Universidad Autónoma de Madrid): *Computational study of azobenzene photoswitches for DNA G-Quadruplex regulation*
- **13:00 - 13:20h:** OC20 - Verònica Postils (University of Bordeaux, France): *Tunning Second-order NonLinear Optical properties through symmetry in Pyrazine Derivatives*

13:20 - 15:15h: LUNCH

SESSION 8a

- **15:15 - 15:35h:** OC21 - Mario Piris (Donostia International Physics Center, Donostia): *Advancements in Natural Orbital Functional Theory: Unraveling Molecular Dynamics and Excited States*
- **15:35 - 15:55h:** OC22 - Josep M. Luis (University of Girona): *Spurious Oscillations along the Nuclear Displacements Caused by Density Functional Approximations*
- **15:55 - 16:15h:** OC23 - David M. Rogers (University of Nottingham): *An Improved Diabatisation Scheme for Computing the Electronic Circular Dichroism of Proteins*
- **16:15 - 16:35h:** OC24 - Tjerk P. Straatsma (Oak Risge National Laboratory, USA): *Computational Chemistry on Exascale Computers: Development of GronOR Non-Orthogonal Configuration Interaction for Fragments*
- **16:35 - 16:55h:** OC25 - Giacomo Ambrogio (Università di Torino, Italy): *GPU Acceleration in First Principle Computational Materials Science for Enhances Efficiency and Scalability*
- **16:55 - 17:15h:** OC26 - Chiara Sepali (Scuola Normale Superiore, Pisa, Italy): *Fully polarizable multiconfigurational self-consistent field/fluctuating charge approach*

SESSION 8b

- **15:15 - 15:35h:** OC27 - Fabiola E. Medina (Universidad del Bío-Bío, Chile): *Reacion Mechanism Exploration of Metallo-β-Lactamase Enzyme via QM/MM Calculations*
- **15:35 - 15:55h:** OC28 - Sérgio F. Sousa (Universidade do Porto, Portugal): *Application of QM/MM Methods in the Study of the Enzyme Efficiency by PET Degrading Enzymes*

- **15:55 - 16:15h:** OC29 - Alejandro Cruz (University of Southern California, USA): *Unravelling GPCRs allosteric modulation. Cannabinoid 1 receptor as case study*
- **16:15 - 16:35h:** OC30 - Lingushu Zhuo (University of Amsterdam, Netherlands): *Ion-assisted CO2ERR in Metal Prophyrin Cage: a DFT study combining static and dynamic modelling*
- **16:35 - 16:55h:** OC31 - Francesca Peccati (Basque Research and Technology Alliance (BRTA), Derio): *Computational Approaches to Enzyme Catalysis: a Critical Assessment of the Preorganization Paragigm in Kemp Eliminases*
- **16:55 - 17:15h:** OC32 - Victor S. Batista (Universitat Jaume I, Castellón): *Study of the polyurethanase activity of lipase RCL by multiscale computational methods*

POSTER SESSION 2

GALA DINNER

Friday, June 7:

SESSION 6:

- **9:00 - 9:45h:** PL8 - Fernando Martin (Univ. Autonoma de Madrid, Spain): *New directions in theoretical attosecond chemistry*
- **9:45 - 10:05h:** IL16 - Anastasia Borschevsky (Univ. of Groningen, Netherlands): *Testing the Standard Model with Molecules*
- **10:05 - 10:25h:** IL17 - Alejandro Gaita-Ariño (Univ. de Valencia, Spain): *A call for frugal modelling: two case studies involving molecular spin dynamics*
- **10:25 - 10:45h:** IL18 - Daniel Roca Sanjuán (Univ. of Valencia, Spain): *Modeling atmospheric chemistry phenomena with strong electron correlation*
- **10:45 - 11:05h:** IL19 - Albert Solé (ICIQ, Tarragona): *Modeling energy transfer processes in photocatalysis*

11:05 - 11:40h: COFFE BREAK

SESSION 7a

- **11:40 - 12:00h:** IL20 - Carme Rovira (Univ. de Barcelona, Spain): *QM/MM studies of protein glycosylation reactions*
- **12:00 - 12:45h:** PL9 - Feliu Maseras (ICIQ, Tarragona, Spain): *Concentration effects in computational homogeneous catalysis*

CLOSURE