III GREGORIO ASENSIO SYMPOSIUM

Friday 16 January 2026

Salón de Grados, Facultad de Farmacia, Universidad de Valencia

PROGRAM

9:45 **Opening**

10:00 **Antonio M. Echavarren**, ICIQ, BIST, Universitat Rovira i Virgili
Molecular Gymnastics through Gold-Carbene Chemistry

10:50 **Sonsoles Martín-Santamaría**, CIB Margarita Salas, CSIC
Multiscale modeling of Toll-like Receptors in Innate Immunity Recognition

11:30 Coffee Break

12:15 **Guillermo Mínguez**, ICMol, Universitat de València
Molten molecular synthesis: an alternative route to unconventional MOFs

12:45 **Ana Belén Cuenca**, IQS, Universitat Ramon Llull
New reactions and structures involving main group elements

13:15 **Daniel Maspoch**, ICN2, BIST, CSIC, Universitat Autònoma de Barcelona
Clip-off Chemistry: breaking bonds, building chemistry

13:45 **Closing remarks**

14:00 Lunch

INSCRIPTION

https://forms.gle/PGhGBWT9WZHh7tF98

* Inscription deadline Monday 12 January.
** Inscription is free for attendants and 30 euros for the lunch.

Molecular Gymnastics through Gold-Carbene Chemistry

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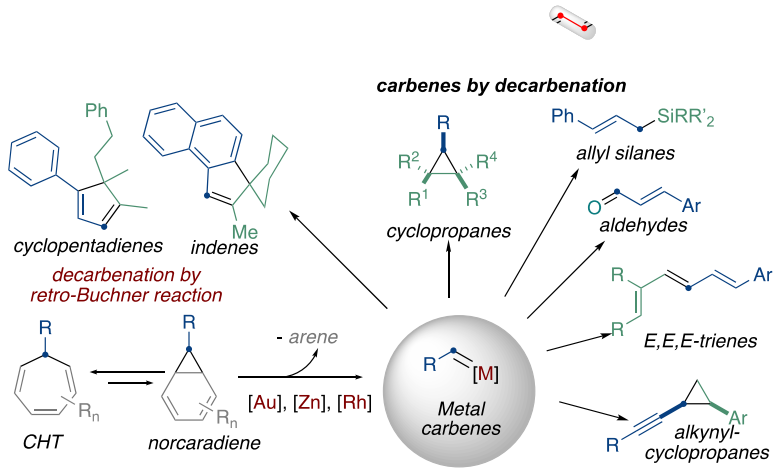
Many gold(I) catalyzed reactions take place through gold(I) carbenes as intermediates.[1,2] Gold(I) carbenes, as well as well as other metal carbenes or carbenoids, can also be generated in solution by retro-Bucher reaction of cycloheptatrienes (formal decarbenation).[3] This lecture will focus on reactions developed in our group that proceed via gold(I) carbenes and related intermediates, leading to the construction of carbon skeletons.[4]



References

1. Jiménez-Núñez, E.; Echavarren, A. M. *Chem. Rev.* **2008**, *108*, 3326–3350. Obradors, C.; Echavarren, A. M. *Acc. Chem. Res.* **2014**, *47*, 902–912.

2. Scharnagel, D.; Escofet, I.; Armengol-Relats, H.; de Orbe, M. E.; Korber, J. N.; Echavarren, A. M *Angew. Chem. Int. Ed.* **2020**, *59*, 4888–4891.

3. Mato, M.; García-Morales, C.; Echavarren, A. M. *ChemCatChem* **2019**, *11*, 53–72. Mato, M.; Montesinos-Magraner, M.; Sugranyes, A. R.; Echavarren, A. M. *J. Am. Chem. Soc.* **2021**, *143*, 10760–10769.

4. Hammarbäck, L. A.; Medina-Gil, T.; Sadurní, A.; Echavarren, A. M. *Org. Lett.* **2024**, *26*, 6375–6379 and refs. therein.

Multiscale modeling of Toll-like Receptors in Innate Immunity Recognition

Sonsoles Martín-Santamaría

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Toll-like receptors (TLRs) sit at the frontline of innate immunity and have emerged as prime therapeutic targets in the era of immunotherapy. Multiscale simulations are applied to the understanding of Toll-like receptors and bacterial infection mechanisms at different levels of organization, where atomistic and coarse-grained models are combined to explore biomolecular interactions. Our research focuses on how TLRs are modulated by small-molecules, glycolipids and lipopolysaccharides, how ligand-specific binding drives TLR dimerization mechanisms, and how antimicrobial peptides disrupt bacterial envelopes to combat infection.

References

i) Pither et al. Angew¡.Chem¡.Int¡.Ed¡.Engl. 2024, 63, e202401541; ii) Matamoros-Recio et al. Carbohydr¡.Polym. 2023, 318, 121094; iii) Franco-González et al. Sci¡. Rep. 2022, 12, 19474; iv) Matamoros-Recio et al. Chemistry, 2021, 27(62), 15406-15425.

Molten molecular synthesis: an alternative route to unconventional MOFs

Guillermo Mínguez Espallargas

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The development of synthetic routes that can combine the high-temperature capabilities of solid-state methods with the kinetic flexibility and diversity of solvent-mediated chemistry is key to accessing materials with unprecedented structures and functionalities. In this sense, molten salt synthesis has been extensively explored, in which inorganic salts such as NaCl provide a high-temperature molten medium that facilitates solid-state transformations while remaining chemically inert. However, its operating temperatures, reaching 1000 °C, is incompatible with systems containing organic molecules.

Herein we present an alternative route to circumvent the need of such high temperatures by the replacement of the molten inorganic salt with a meltable organic molecule, and we will show the applicability of this uncommon synthetic approach in the field of metal-organic frameworks (MOFs). We will present the preparation of elusive porous crystalline materials such as the iron(II) analogue of ZIF-8,[1] and multivariate analogues.[2,3] We will also show the applicability of the molten molecular synthesis to prepare crystalline precursors that can be converted in MOF-derived glasses,[4-6] and finally, the use of this synthesis to prepare MOF-derived glasses a direct way.[7]

References

[1] J. López-Cabrelles, et al. *J. Am. Chem. Soc.* **2019**, *141*, 7173.

[2] J. López-Cabrelles, et al. *Chem. Sci*. **2022**, *13*, 842.

[3] L. León-Alcaide *et al. J. Am. Chem. Soc.* **2023**, *145*, 23249.

[4] L. León-Alcaide *et al. J. Am. Chem. Soc.* **2023**, *145*, 11258.

[5] L. León-Alcaide *et al. Chem. Commun*. **2025**, *61*, 11641.

[6] L. León-Alcaide *et al. Chem. Sci*. **2025**, *16*, 7946.

[7] L. León-Alcaide *et al. Nat. Commun.* **2025**, *16*, 8783.

Clip-off Chemistry: breaking bonds, building chemistry

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Historically, innovations in synthetic methods and chemical reactions have transformed how scientists design and synthesize molecules and materials. Indeed, novel reactions or synthetic strategies not only enable access to previously unattainable structures but also inspire new paradigms for constructing materials that address global social, economic, and industrial challenges.

In this talk, I will introduce the concept and recent advances in Clip-off Chemistry. This approach is based on the design and synthesis of novel molecules and materials with well-defined compositions and structures via bond cleavage within molecular frameworks. Clip-off Chemistry thus represents a new synthetic methodology in which programmed, selective disassembly leads to the formation of new molecules and materials. This molecular disassembly is achieved through chemical reactions; in a first approach, via ozonolysis, which enables the cleavage of organic building blocks or linkers through direct breaking of alkene or alkyne bonds. I will present the fundamental principles of Clip-off Chemistry and recent examples of molecules and structures obtained through controlled bond fission in porous reticular materials.