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CiQUS Lecture

**Supramolecular Nanocapsules
as Masks for Regioselective
Functionalization
of Fullerenes****April 3, 2025**

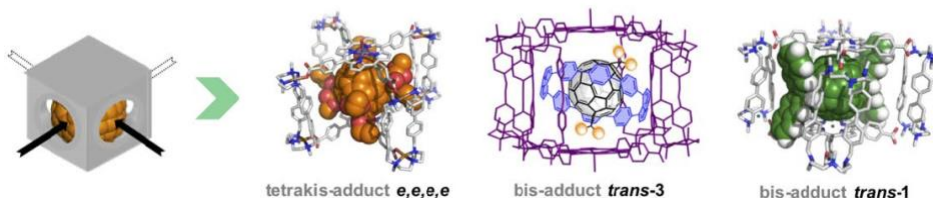
CiQUS Seminar Room | 6 PM

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Abstract

The regioselective functionalization of fullerenes and the control of the number of adducts is highly important to unbar the development of fullerene chemistry. Nowadays, easy-accessible C₆₀ and C₇₀ fullerene mono-adducts are mainly used in any application^[1] due to the hampered accessibility to pure alternative fullerene poly-adduct derivatives. In a general basis, multi-adduct mixtures with uncontrolled regioselectivity (multi-isomers) are obtained, and chromatographic purification is too costly and time consuming to be used in the synthesis of multiadduct fullerene species. Herein, porphyrin-based supramolecular nanocapsules^[2,3] are used as supramolecular shadow masks to tame the over-reactivity of Bingel-Hirsch-type cyclopropanation reactions and, more importantly, to have full control on the equatorial regioselectivity and on the number of additions. Thus, exclusively equatorial bis-, tris- and tetrakis-C₆₀ adducts using ethyl-bromomalonate are stepwise obtained and fully characterized (NMR, UV-vis and XRD). Furthermore, the regioselectivity control is finely tuned using a three-shell Matryoshka-like assembly towards the synthesis of a single trans-3 bis-Bingel-C₆₀ for the first time.^[4] Also, the mask strategy is extended to Diels Alder reactions with full control of the regiolectivity in the synthesis of trans-1 bis-pentacene-C₆₀.^[5] These results, recently extended to C₇₀,^{[6][7]} are fully attributed to the confinement control imposed by the capsule's cavity, and represent a novel and unique strategy to infer regiocontrol to the synthesis of fullerene multi-adducts. We envision that the described protocol will produce a plethora of derivatives for applications such as solar cells.

Supramolecular Masks**References:**

1. E. Castro, L. Echegoyen et al. J. Mater. Chem. C, 2018, 6, 2635.
2. C. García-Simón, X. Ribas, et al. Nat. Commun. 2014, 5:5557.
3. C. Fuertes-Espinosa, X. Ribas, et al, Chem 2020, 6, 169–186.
4. E. Ubasart, X. Ribas, et al, Nat. Chem. 2021, 13, 420-427.

5. M. Pujals, X. Ribas, et al, Cell Rep. Phys. Sci. 2022, 3, 100992.
6. V. Iannace, X. Ribas et al, J. Am. Chem. Soc. 2024, 146, 5186–5194.
7. T. Pèlachs, X. Ribas et al, CCS Chem 2025, 7, 703–715.

Biosketch

Xavi Ribas (1974, Santa Coloma de Farners) obtained his PhD in Chemistry at the University of Girona (UdG) in 2001, and he carried out a 3-year postdoc at ICMAB-CSIC in 2002-2004. He was promoted to Associate professor in Chemistry at UdG in 2006. His research over the last years has been focused on three main projects; a) Fundamental mechanistic studies on redox transition metals in organometallic cross coupling and C-H activation and functionalization of arenes, b) Study of structural and functional modelling of non-heme Fe, Mn and Cu oxygenases and its application as selective oxidation catalysts, c) development of nanocapsules for catalysis at the confined space, host-guest reactions and purification of fullerenes and endohedral metallofullerenes (EMFs).

He was awarded with an ICREA-Acadèmia prize in 2010, and an ERC-Starting Grant in 2011 (ERC-2011-StG-277801, till Nov 2017), the latter on C-X and C-H functionalization involving Cu(III) species. Moreover, he obtained two consecutive grants from MINECO (CTQ2013-43012-P, CTQ2016-77989-P). He was awarded with a second ICREA-Acadèmia prize in 2015, and an ERC-Proof of Concept Grant in 2015 (ERC-PoC-2015-709590). He is also leading the Catalan project (2017 SGR 264), and the Univ. Girona research projects MCPuDG2016 and GdRCompetUdG2017. In 2018 he was awarded with the Premio a la Excelencia Investigadora RSEQ 2018.

His work has been published in 123 articles in peer reviewed journals. Moreover, he published 5 book chapters, filled 5 Spanish patents and he edited the book entitled "C-H and C-X functionalization. Transition metal mediation", published by RSC-Publishing in 2013. He has communicated his work in more than 170 international conferences and he has given over 45 lectures at international conferences and universities. He is also the co-founder of the SpinOff company GIOXCAT.