

# SEMINAR

## MONDAY 20<sup>TH</sup> MAY 11:30 – ROOM G

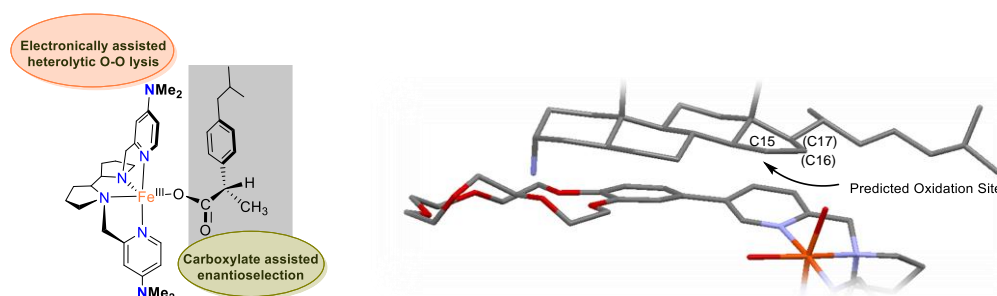
### Prof. Miquel Costas

### Ciamician-Gonzales Lecturer 2024

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## Site and Enantioselective Oxidation of Strong C–H Bonds with Bioinspired Catalysts

Nature is a source of inspiration for the development of chemical transformations that stand as unsolved problems in contemporary synthetic chemistry and also for creating sustainable alternatives to methods that are becoming increasingly prohibitive because of society needs to change from a linear to a circular economy. Reaction mechanisms and reagents operating in metalloenzymes can be the starting point guiding the design of small molecule catalysts based in well-defined coordination compounds that retain the main chemical reactivity features of the enzyme while avoiding the size and complexity inherent of the protein scaffold.<sup>1</sup> Coordination complexes can reproduce fundamental aspects of the chemistry of oxygenases and can be powerful oxidation catalysts;<sup>2</sup> upon reaction with hydrogen peroxide, high valent metal-oxo species are formed that can engage in C–H oxidation reactions proceeding via short lived radical intermediates. Control of the first and the second coordination sphere of the catalysts can be used to shape the place where the metal-oxo reactive center attacks the C–H bond, and this translates into site and stereoselective C–H oxidation reactions.<sup>3</sup> Strategies pursued for the design of biologically inspired catalysts based on the manipulation of electronic and steric properties of the catalysts, and incorporation of substrate recognizing units via supramolecular effects will be discussed.<sup>4,5</sup>



*Strategies to pursue selective C–H oxidation; left) steric and electronic manipulation of the catalyst. Right) weak interactions with substrate recognition units.*

#### References

- 1) White, M. C.; Zhao, J. *J. Am. Chem. Soc.* **2018**, *140*, 13988.
- 2) Vicens, L.; Olivo, G.; Costas, M. *ACS Catal.* **2020**, *10*, 8611.
- 3) Costas, M. *Chem. Rec.* **2021**, *21*, 4000.
- 4) a) Cianfanelli, M.; Olivo, G.; Milan, M.; Klein Gebbink, R. J. M.; Ribas, X.; Bietti, M.; Costas, M. *J. Am. Chem. Soc.* **2020**, *142*, 1584.  
b) Vicens, L.; Bietti, M.; Costas, M. *Angew. Chem. Int. Ed.* **2021**, *60*, 4740.
- 5) a) Vicens, L.; Olivo, G.; Costas, M. *Angew. Chem. Int. Ed.* **2022**, *61*, e202114932. b) Olivo, G.; Capocasa, G.; Ticconi, B.; Lanzalunga, O.; Di Stefano, S.; Costas, M. *Angew. Chem. Int. Ed.* **2020**, *59*, 12703–12708.

All the interested people are invited to attend

Alceo Macchioni