MD3dCAT

Mechanism-driven Design of 3d Transition Metal Catalyzed CH Functionalization Reactions

Timeline | 09/2021 to 08/2024

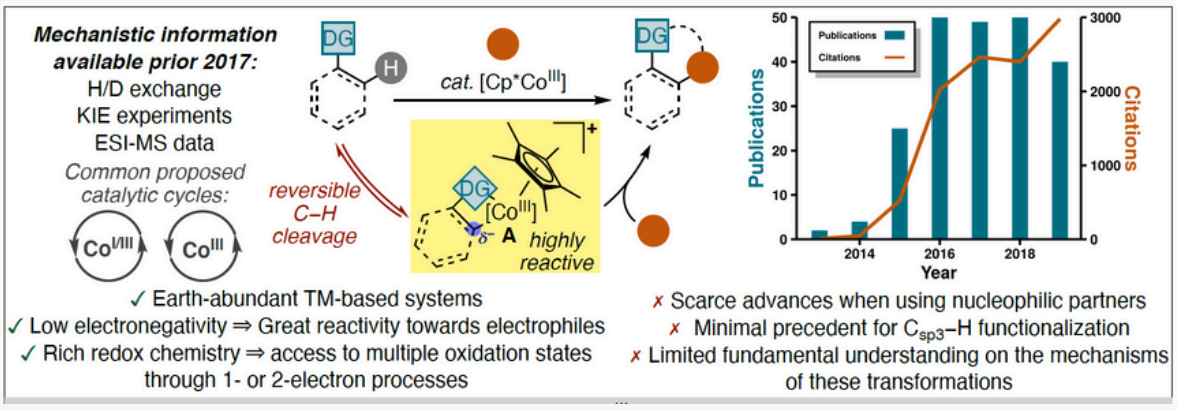
Budget | 157,300 €

ICIQ People | Mónica Pérez-Temprano Research Group

Call | Proyectos I+D - Generación Conocimiento 2020

SUMMARY

The selective conversion of C-H bonds into carbon-carbon and carbon-heteroatom bonds constitutes an ideal method for the rapid and efficient construction of pharmaceuticals, agrochemicals or polymers. During decades, this fields has been dominated by the employment of catalysts based on noble metals such as Pd, Rh or Ir. Despite over the past years first-row transition metals, more abundant and inexpensive, have emerged as a very attractive alternative to these precious metals, these 3d-based systems are still at their infancy, not only due to major synthetic limitations but also due at the fundamental level. In most cases, there is a lack of fundamental knowledge on how these transformations occur which hampers the development of more efficient and innovative catalytic reactions. This project, **MD3dCAT**, offers a unique opportunity for streamlining the sustainable synthesis of organic scaffolds of relevance for different fields, including medicinal chemistry. To do so, we will use fundamental knowledge as the center of process design for developing more sustainable processes and unlocking unprecedented reactivity patterns in the context of site-selective C-H functionalization reactions by using different cobalt and manganese catalysts. The proposed strategy provides practical and versatile solutions for enhancing the sustainability of chemical processes.



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Reference: PID2020-112733GB-I00/MICIU/AEI/10.13039/501100011033