Deciphering Mechanisms to Design Better Catalytic Reactions

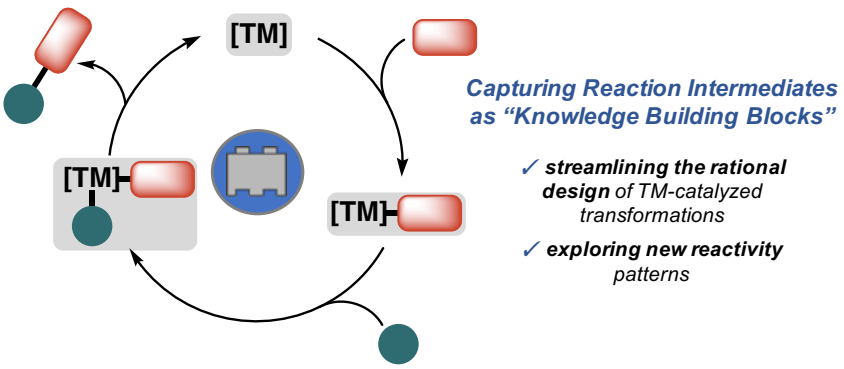
Mónica H. Pérez-Temprano

Institute of Chemical Research of Catalonia (ICIQ) Av. Països Catalans, 16 43007 Tarragona (Spain)

mperez@iciq.es

Most reactions set-up in the lab fail.[1] This is one of the biggest problems chemists faces when designing transition metal-catalyzed transformations.[2] This striking situation prompts two key questions: Why do reactions fail? Can failed reactions be used to trigger a paradigm-shift in reaction design?

My group aims to answer these questions placing fundamental understanding at the center of process design. We use mechanistic studies as a powerful tool to facilitate the bottom-up design of more efficient chemical processes.[3] My research program is based on simple, yet usually overlooked, concept: chemical reactions rely on the performance of the reactive intermediates within the catalytic cycles. By capturing these transient species and using them as "knowledge building blocks" (KBBs), we expose the obstacles hindering transition metal-catalyzed transformations efficiency and capitalize on the gathered fundamental knowledge to streamline more resource-efficient transformations. As a proof-of-concept, my group targets chemical transformations catalyzed by cost-effective cobalt complexes.[4]



(1) Zaragoza Dörwald, F. Side Reaction in Organic Synthesis: A guide to Successful Synthesis Design. Wiley- VCH Verlag GmbH&Co. 2005.
(2) Collins, K. D.; Glorius, F. *Nat. Chem.* **2013**, *5*, 597.
(3) Sanjosé-Orduna, J.; Mudarra, A. L.; Martínez de Salinas, S.; Pérez-Temprano, M. H. *ChemSusChem* **2019**, *12*, 2882.
(4) (a) Sanjosé-Orduna, J.; Gallego, D.; Garcia-Roca, A.; Martin, E.; Benet-Buchholz, J.; Pérez-Temprano, M. H. *Angew. Chem. Int. Ed.* **2017**, *56*, 12137. (b) Sanjosé-Orduna, J.; Sarria Toro, J. M.; Pérez-Temprano, M. H. *Angew. Chem. Int. Ed.* **2018**, *57*, 11369. (c) Martínez de Salinas, S.; Sanjosé-Orduna, J.; Odena, C.; Barranco, S.; Benet-Buchholz, J.; Pérez-Temprano, M. H. *Angew. Chem. Int. Ed.* **2020**, *59*, 6298. (d) López-Resano, S.; Martínez de Salinas, S.; Garcés-Pineda, F. A.; Moneo-Corcuera, A.; Galán-Mascarós, J. R.; Maseras, F.; Pérez-Temprano, M. H. *Angew. Chem. Int. Ed.* **2021**, *60*, 11217.