CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES:
Advancing light-mediated Ni catalysis using data science and physical organic techniques

Abstract:

The Bahamonde group harnesses the distinct one-electron chemistry and photochemical reactivity of Ni complexes to generate and trap C-centered radicals enantioselectively and promote C−N reductive eliminations at room temperature. Our excitement for studying these systems stems from the fact that these two apparently unrelated processes are facilitated under almost identical conditions, but to date the ligand features, photocatalyst properties, and subtle reaction condition variations that favor one pathway over the other are not yet understood. Additionally, to expedite reaction optimization, the group develops multivariate linear regression models correlating observed enantioselectivity to computed molecular descriptors.

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About the Speaker:

Ana was born in the north of Spain in 1989. She obtained her B. Sc. in Chemistry at the Universidad de Oviedo in 2012. Subsequently, during her PhD she studied photoredox reactions promoted by organocatalysts at the Institute of Chemical Research of Catalonia (ICIQ). Afterwards she moved away from her home country to work as a postdoctoral researcher at the University of Utah (2017-2020) where she worked on Pd-catalyzed aza-Wacker reactions and the development of multivariate linear regression models to explain the rates of amide coupling reactions. Currently, she is an Assistant Professor at the University of California Riverside where her group uses a mechanistically guided approach to reaction development utilizing first row transition metals.