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DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE SEMINAR SERIES FALL 2022

WEDNESDAY, OCTOBER 26, 2022

VIRTUAL

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1:00PM-2:20PM

GUEST SPEAKER

Cristina Trujillo, PhD Lecturer in Computational & Theoretical Chemistry Department of Chemistry The University of Manchester <u>https://trujilloresearchgroup.com</u> @Trujillo_Group

TOPIC

Mechanistic Insights and Prediction in Organocatalysis - A Computational Approach

ABSTRACT

Organocatalysis remains one of the most challenging topics in contemporary organic chemistry. While the symmetric and asymmetric organocatalysis fields currently is growing exponentially, an understanding of the mechanistic details involved in most of these reactions has often lagged far behind the pace of catalyst development, which retards catalyst design. However, over the last two decades, computational methods have become a cost-effective treatment of large chemical systems with reasonable accuracy to provide a rationale for the experimental outcome. In this seminar, computational studies in organocatalysis underpinning stereochemical results, mechanisms and binding modes will be discussed. This talk will include two different topics, firstly the base-catalysed Tamura cycloaddition between homophthalic anhydride and activated alkenes/alkynes will be discussed, a joint experimental–computational study to establish the mechanism of the base-catalysed Tamura cycloaddition. And secondly, a full theoretical study on the computationally-led design of catalysts within phase transfer catalysis will be presented.

The delicate balance between sterical and attractive Non-Covalent Interactions (NCIs) as the main controlling factors in organocatalysis will be examined.



BIO



Dr. Cristina Trujillo obtained her doctorate in Theoretical and Computational Chemistry in 2008 at the Universidad Autónoma de Madrid (Spain). During the period 2008-2016, she held several Postdoctoral positions in Spain (CSIC), Prague (Academy of Sciences), and Ireland (Trinity College Dublin). From 2016 until 2018 she worked at TCD as a Research Fellow. After postdoctoral training, she worked as an Assistant Lecturer in TU-Dublin in the School of Chemical & Pharmaceutical Sciences. She subsequently was awarded the very competitive SFI-Starting Investigator Research Grant (SIRG, 2018) and L'Oreal-Unesco Women in Science UK and Ireland Fellowship -Highly Commended (2019). She worked as an independent researcher leading her research group

at TCD from 2019 to 2022. Currently, she is a Lecturer in Computational & Theoretical Chemistry at The University of Manchester.

She has expertise in highly fundamental topics within Computational Organic Chemistry such as asymmetric catalysis, computationally-led catalysis design, mechanisms of reaction, and noncovalent interactions. Her research interests are focused on the asymmetric catalysis field, with particular emphasis on the application of computational techniques in the design of organocatalysts along with prediction and control of catalytic processes, with a direct impact on the development of products with different applications.

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