



Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

Dr. Cristina Trujillo
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PhD in Computational Organic Chemistry

Overview: A fully SFI-funded PhD studentship is available in the School of Chemistry, Trinity College of Dublin within Dr. Cristina Trujillo research group. This project is framed within the field of computational organic chemistry focusing on the application of the best computationally-design models that impact directly on the development of important pharmaceutical products.

Project Description: The *objective* of this project is to carry out a thorough computational study leading to the understanding of the potential for nucleophilic catalysis in a chiral environment to be applied to synthetically useful transformations. This study is part of a wider research project focused on nucleophilic catalysis *via* fluoride and the design of new organocatalysts using computational chemistry tools (based on quantum chemistry theory). Those new organocatalysts will be used to design new, green and non-toxic procedures for obtaining a wide range of pharmaceutical compounds.

Requirements: Applications are welcome from students from Ireland/EU with, or expecting to gain, a first class honours degree, or equivalent, in Chemistry, or a related subject, and who can demonstrate an interest in both computational and organic chemistry. Some experience in computational methodologies (i.e. DFT and MP2) would be advantageous, although training will be provided. The candidate must be highly motivated and able to work both independently and as part of a supportive team. Excellent communication and organisational skills are also required. The successful candidate will be part of the Dublin Chemistry programme and attend to group meetings, seminars and international conferences. The student will develop advanced computational and organic chemistry skills.

Application: The position is fully funded (stipend & fees) and will be part of the Dublin Chemistry Graduate Programme. The **deadline** for applications is **31th May 2019**. The expected **start date is October 2019**. To apply please email a PDF copy of a brief cover letter and CV to trujillc@tcd.ie.

Informal enquiries before the application deadline are welcomed and may be addressed to Dr Cristina Trujillo (trujillc@tcd.ie).