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PhD project: **materials design of photocatalysts for $CO_2$ conversion to added-value chemicals**

Applications are invited for a Queen Mary University of London – China Scholarship Council PhD studentship starting in October 2021 to work in the laboratories of *Dr Rachel Crespo-Otero* and *Dr Devis Di Tommaso* at the Department of Chemistry.

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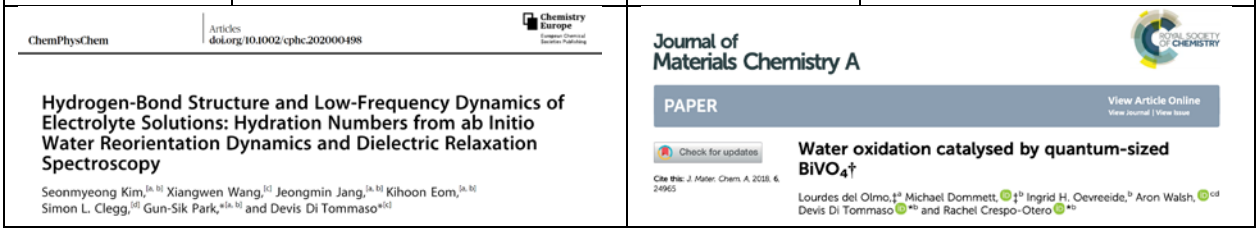
| Di Tommaso lab | ✓ Ab initio molecular dynamics<br>✓ Statistical thermodynamics<br>✓ $CO_2$ reduction and mineralization | Crespo-Otero lab | ✓ Excited state dynamics<br>✓ Computational photochemistry<br>✓ Method development and programming |




**Context.** The rising level of carbon dioxide ($CO_2$) in Earth's atmosphere caused by the excessive emission from fossil fuel is the main cause of global warming. The development of efficient technologies for the capture and utilization of atmospheric $CO_2$ represent a huge challenge, but also an opportunity. One of the most attractive strategies to reduce fossil fuel consumption and climate-changing emissions would be to convert $CO_2$ into low carbon fuels. Such a strategy can reduce the accumulation of $CO_2$ in the atmosphere, produce useful chemicals, thus relieving our dependence on conventional fossil resources.

**Project.** The successful candidate will conduct of atomistic simulations for the design of sustainable photo-catalysts, that could efficiently facilitate the conversion of $CO_2$ to value-added chemicals. The student will be trained in excited state modelling, DFT and *ab-initio* techniques and molecular dynamics techniques. Transferable skills such as the design of modular computer codes will also be developed. The project will be conducted in collaboration with experimental groups at Queen Mary University (*Dr Jorge Sobrido* and *Dr Giordano*) and Tohoku University (*Prof. Nishihara*).

The successful candidate will benefit from our membership to the Thomas Young Centre (TYC), the centre for the theory and simulation of materials and modelling, gathering together researchers from UCL, Imperial, KCL and QMUL. Dr Crespo-Otero and Dr Di Tommaso are Co-Directors of the TYC. Their group have access to *outstanding* university, regional and national high-performance computing facilities. The student will have the opportunity for regular travel to UK national and international conferences to present their work and will be expected to publish high impact scientific publications.

**Requirement.** Applications are invited from candidates with, or expecting to be awarded, an MSc degree in the areas of physical chemistry, theoretical chemistry, materials sciences and physics. Applicants are required to provide evidence of their proficiency in English language skills. For further entry requirements and to apply, please follow the link. Applicants are encouraged to contact Dr Crespo-Otero (r.crespo-otero@qmul.ac.uk) or Dr Di Tommaso (d.ditommaso@qmul.ac.uk) prior to their submission by sending a CV and cover letter describing their research interests and expertise, and the names of two referees.