# MIGUEL RIVERA

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Computational Chemistry Lecturer (Teaching). Fast learner with experience in communication and collaborative work environments.

#### **SKILLS**

# • Programming

- Expert in Python with five years of experience, and providing programming support within my research group.
- Experience working with Fortran and C/C++ legacy research codes, adapting them and refactoring them which made them useable in my group's in-house research.
- Experience scripting in bash and perl.

#### • Best Practices

- Led the development of an open source programming library (fromage).
- Wrote technical documentation for my open source project using Read the Docs.
- Experience fostering an open source project community, presenting talks and posters at conferences which resulted in external research groups using my software.
- Proficiency in designing and planning test-driven development, thanks to self-teaching of:
  - \* Version control with Git
  - \* Unit testing with pytest
  - \* Continuous integration with TravisCI
  - \* Code quality control with LGTM

### • High-Performance Computing

- Worked on national, regional, and institutional computer clusters using MPI, and OpenMP.
- Used a Linux desktop as a principal work computer for five years, making me very comfortable with maintining Unix-like systems.

# • Numerical Simulations

- Generation and organisation of high dimensional and correlated data in the form of computational simulations of quantum systems and the study of their application for eco-friendly, cheap, and flexible light-interacting materials.
- Development of hybrid modelling schemes which combine pre-existing quantum simulation methods which now allows for the modelling of previously under-researched materials.

#### • Data Science

- Two in-progress publications applying newly developed modeling methods to large numbers of chemical systems, using regression analysis to aid materials design.
- Two publications on chemical theory based on comparison with experiment, advancing the field of optical technology.
- Personal project neural network experience with Kaggle using Keras.

#### • Communication

- Six publications at different stages of completion, three as lead author, presented at multiple conferences.
- Trained three graduate research students to use computational chemistry software, including my own.
- Volunteered to demonstrate computational research techniques to year thirteen students at the Queen Mary Summer School.
- Attended the Hermes Summer School 2018 with a focus on science communication.

#### Miscellaneous

- Fluent in English, French, and Spanish.
- User of vim, LATEX, Inkscape, and MS Office.
- Data visualisation with matplotlib, seaborn, Jupyter and gnuplot.
- Image manipulation using Inkscape and GIMP.
- Worked in a cross-disciplinary group of 3-8 members with different levels of experience.

#### PROFESSIONAL EXPERIENCE

UCL
Lecturer (Teaching) in Computational Chemistry

Imperial College London
Research Assistant in the Department of Materials

Queen Mary University of London
Doctoral researcher in Methods for Photochemistry in Molecular Crystals

Queen Mary University of London
Teaching demonstrator in Computational Chemistry and Introduction to Scientific Programming

The Happy Hour Collective

02/2022 - present
04/2020 - 01/2022
01/2020 - 01/2022
01/2020 - 01/2022
01/2016 - 03/2020
01/2017 - 03/2020
01/2017 - 03/2020
01/2017 - 03/2020

# REPRESENTATIVE PUBLICATIONS

Semi-professional guitarist for a jazz function band

ONIOM(QM:QM') Electrostatic Embedding Schemes for Photochemistry in Molecular Crystals

- Miguel Rivera, Michael Dommett, and Rachel Crespo-Otero

Journal of Chemical Theory and Computation 2019 (preprint)

Fromage: A Library for the Study of Molecular Crystal Excited States at the Aggregate Scale

- Miguel Rivera, Michael Dommett, Amir Sidat, Warda Rahim, and Rachel Crespo-Otero Journal of Computational Chemistry 2020 (preprint) Molecular and Crystalline Requirements for Solid State Fluorescence Exploiting Excited State Intramolecular Proton Transfer

- Michael Dommett, **Miguel Rivera**, Matthew T. H. Smith, and Rachel Crespo-Otero Journal of Materials Chemistry C 2020 (preprint)

## **AWARDS**

2 Talk prizes	Material Research Institute 2018, Thomas Young Centre Student Day 2018
2 Poster prizes	Computational Molecular Science 2019, Molecular Quantum Mechanics 2019
5 Grants	Computing time from Materials Chemistry Consortium, total $\sim £2500$

# **EDUCATION**

Queen Mary University of London, UK	10/2016 - 04/2020
PhD in Computational Chemistry with Rachel Crespo-Otero	
University College London, UK	10/2012 - 05/2016
MSci in Physics with David Bowler	
Lycée International des Pontonniers, Strasburg, France	09/2009 - 07/2012
French Baccalaureate with International Option in English	