

MIGUEL RIVERA

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Computational Chemistry PhD graduate with numerical and programming skills, interested in working in meaningful challenges in programming and research. 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 maintaining 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, L^AT_EX, 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

Queen Mary University of London

10/2016 - present

Doctoral researcher in *Methods for Photochemistry in Molecular Crystals*

Learning

- Transitioned from a Physics background to a Chemistry research department where I was required to learn highly specialised chemical methods within weeks to meet deadlines.

Queen Mary University of London

01/2017 - present

Teaching demonstrator in *Computational Chemistry* and *Introduction to Scientific Programming*

Teaching

- Assisted in the development of a new Python course in the department where all of the 196 students passed the class in the year 2018-2019.

The Happy Hour Collective

12/2014 - present

Semi-professional guitarist for a jazz function band

Interpersonal Skills

- Communicated with clients and audiences in a professional environment, resulting in 15 paid performances across the UK.

REPRESENTATIVE PUBLICATIONS

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 ~ £2500

EDUCATION

Queen Mary University of London, UK

10/2016 - present

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