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 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

Imperial College London *04/2020 - present*
Research Assistant in the Department of Materials

Queen Mary University of London *10/2016 - present*
Doctoral researcher in *Methods for Photochemistry in Molecular Crystals*

Queen Mary University of London *01/2017 - present*
Teaching demonstrator in *Computational Chemistry* and *Introduction to Scientific Programming*

The Happy Hour Collective *12/2014 - present*
Semi-professional guitarist for a jazz function band

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 $\sim$ £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