# Alexander Punter

DOB: 20/05/1991 | ajpunter@gmail.com

## **EDUCATION**

### **AIX-MARSEILLES UNIVERSITY**

PHD IN CHEMICAL SCIENCES
Oct 2019 | Aix-Marseilles University,
France

### **DURHAM UNIVERSITY**

MPHYS IN THEORETICAL PHYSICS Aug 2013 | Durham, UK

### KING EDWARD'S SCHOOL

Aug 2009 | Bath, UK

### LINKS

Github://cvzj57 LinkedIn://alexander-punter

### ACADEMIC FOCUSES

### **DOCTORAL**

Quantum Chemistry Computational Chemistry Hartree-Fock Theory Density Functional Theory Computational Modelling Numerical Methods

### **UNDERGRADUATE**

Quantum & Classical Physics Condensed Matter Physics Astrophysics Theoretical Physics Functional Programming

### **SKILLS**

### **PROGRAMMING**

Python • Shell • Django • Git • Subversion • Latex • gnuplot • Javascript • SQL • Docker • Selenium • Sikuli

# QUANTUM CHEMISTRY SOFTWARE

Turbomole • GAMESS • Molden • VMD

### **OTHER**

French (approximately B2 level) • Full UK Driving License

# INTERESTS

Playing music (violin) • Reading (fiction & non-fiction) • Language-learning (French & Mandarin) • Motorcycling

# RELEVANT EXPERIENCE

### **AIX-MARSEILLES UNIVERSITY | DOCTORAL STUDENT**

Sep 2016 - Nov 2019 | Marseilles, France

- PhD Title: 'Molecular Pseudopotentials for the study of Molecular Properties'
- Supervisors: Dr Yannick Carissan & Dr Paola Nava, CTOM group
- Developed a pseudopotential method for the replacement of small carbon fragments in molecular calculations.
- Analysed the performance of this method across a wide variety of molecules and properties.
- Wrote the MOO program to facilitate the easy use of these pseudopotentials, as well as the optimisation of new ones. This was done in Python and interfaced with the TURBOMOLE package.
- Also worked on establishing reaction mechanisms for Cobalt complexes.
- Conference Presentations: Annual Northern Universities Meeting on Chemical Physics 2019, Francophone Theoretical Chemists' Conference 2018
- Conference Posters: International Conference on Quantum Chemistry 2018, Winter School in Theoretical Chemistry 2018, CECAM DFT School 2017

### **TURNITIN UK | QA ASSOCIATE**

Jan 2016 - Jul 2016 | Newcastle, UK

- Tested various parts of the Turnitin software on multiple platforms (Blackboard, Moodle) both manually and through automated teste suites. This work was done primarily in Python (via Selenium) with some Java.
- Worked in an Agile development team.
- Tested both general functionality and compliance with W3C Accesibility guidelines.

### JOINERYSOFT | JUNIOR DEVELOPER

Oct 2013 - Dec 2015 | Shepton Mallet, UK

- Developed an automated test framework for the Joinerysoft package, as well as a web interface. This involved working extensively with Python, Django and Sikuli.
- Worked as a general developer on the JMS4 package. This involvedwork in Python, Django and Javascript.

### **DURHAM UNIVERSITY | UNDERGRADUATE**

Sep 2009 - Aug 2013 | Durham, UK

• Master's Project: 'The Modelling of Active Galaxies' A mathematical and computational project to derive a velocity law describing the mass outflow from Active Galactic Nuclei, with a simulated spectrographic datacube to compare with real data. This was done in Python and matplotlib.

# **PUBLICATIONS**

2019	Int. J. Quantum Chem.	Atomic pseudopotentials for reproducing $\pi$ -orbital electron behavior in $sp^2$ carbon atoms
2019	Dalton Transactions	When Cobalt-Mediated [2+2+2] Cycloaddition Reaction Dares Go Astray: Synthesis of Unpre- cedented Cobalt(III)-Complexes
Submitted for review	-	Pseudopotential-Fragment Spectroscopy for Organic Molecules and Carbon Allotropes

# VOLUNTEER WORK

Project VOICE	Finance & Technical Support 2016-current	Proofreader, typesetter, graphic designer, website maintenance, accounting.
St John Ambulance	Volunteer	Covered events around the country, both as a first aider and an ambulance attend-
	2009-2016	ant.
St John Ambulance	Unit Finance	
	Officer	Managed finances for budgeting, equipment and training.
	2011-2013	
St John Ambulance	Heartstart	
	Co-ordinator 2010-2011	Organised and ran charity and commercial first aid courses.