# Calum Hand

Bath, United Kingdom

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Skills \_\_\_\_\_

**Research** Design & analysis of experiments, Project management, Critical evaluation, Cross-disciplinary mindset

Machine Learning & Cheminformatics Scikit-learn, RDKit, Deepchem, GPy, GPFlow, Data visualisation

Programming & Development Python, OOP, Version control, Continuous integration, Automated testing, Environment Management

Education \_

EPSRC Centre for Sustainable & Circular Technologies - University of Bath

Integrated PhD & MRes Sept 2018 - Present

SUSTAINABLE CHEMICAL TECHNOLOGIES (CHEMICAL ENGINEERING)

Applying machine learning to accelerate in-situ discovery of highly performant materials

MRes (Distinction)

GREEN CHEMISTRY Sept 2016 - Aug 2017

Conducted year long project on synthesis of novel organic molecules

BSc (2.1)

Sept 2012 - June 2016

**University of St. Andrews** CHEMISTRY WITH MEDICINAL CHEMISTRY

Imperial College London

Attended workshops given by AtraZeneca and GSK on their drug discovery process

### Research Experience \_\_\_\_\_

#### **Sustainable Circular Technologies**

Integrated PhD & MRes

Sept 2018 - Present

University of Bath - Centre for Sustainable & Circular Technologies

"Bayesian Screening: Multi-test Bayesian Optimization Applied to in silico Material Screening" (arXiv:2009.05418)

- "Autonomous Exploration and Identification of High Performing Adsorbents using Active Learning" (ChemRxiv: 10.26434/chemrxiv.14555706.v1)
- · Developing a significant Python package, integrating active learning and molecular simulations for novel screenings
- Development of novel graph featurisation methods for materials in machine learning applications
- Work extensively with popular libraries like scikit-learn, including writing novel models / data transformers

**Green Chemistry** MRes (Distinction)

IMPERIAL COLLEGE LONDON

Sept 2016 - Aug 2017

- Successfully demonstrated bio-renewable materials utilisation as a synthetic precursor for solar cells
- · Research combined DFT calculations and novel synthetic strategies to investigate and synthesise target materials
- · Granted a high degree of autonomy, allowing development of strong, self-motivated research ethic

#### **Chemistry with Medicinal Chemistry**

BSc (2.1)

University of St. Andrews

Sept 2012 - June 2016

- "The synthesis of Hibbert ketone structures in technical lignins" (Org. Biomol. Chem., 2016, 14, 10023 10030) Year long project investigating the synthesis of small molecules

## Professional & Work Experience \_\_\_\_\_

**Co-forest Ltd** Bath IKEEP COLLABORATOR Feb 2021

· Worked as part of three person "intrapreneurial" knowledge exchange program between local business and PhD researchers

- · Project involved creating a plan to establish sense of community within "Co-forest" public and industrial clients
- · The outcomes of this collaboration included the identification of company goals in order to create content for specific customers and the drafting of relevant promotional materials.

#### RIMES Technologies (Financial data management)

London

ACCOUNT TEAM MEMBER Sept 2017 - Aug 2018

- Initially hired as part of a global team of analysts. Daily tasks included: being first point of contact for all of RIMES'300 clients; efficiently analysing anomalies within client's data; and identifying and fixing errors within RIMES' in house coding language
- Due to my proficiency in problem solving, knowledge of the RIMES tools and experience with clients, I was promoted to the account team of RIMES' largest client after only six months
- This promotion allowed me to work on the more technical and challenging problems being faced by the client including working on the development and implementation of their new data feed system, the largest single project RIMES had undertaken in their company history
- · Routinely worked across multiple departments requiring me to be an effective communicator for both clients and technical teams
- Due to the fast paced nature of the role, an ability to prioritise tasks and often work on multiple issues at once was a key skill I developed while at RIMES

The Big Issue Glasgow

**OUTREACH & OFFICE VOLUNTEER** 

July 2016 - Sept 2016

- Travelled extensively within the West of Scotland in order to help and build relationships with street vendors about problems they were experiencing relating to their work, and offering support to vendors who had experienced abuse or been victim to violent crime
- · Assisted with the sale of magazines to vendors, allocating vending pitches for the week and ensuring records were maintained and up to date

#### YMCA Camp Silver Beach

USA - Virginia

ALPINE TOWER STAFF & COUNSELLOR

May 2015 - Aug 2015

- Worked as staff for the rock climbing tower and counsellor to cabin of 13 campers
- We were responsible for setting up and maintaining all equipment used on the tower and zipline every day and making sure all equipment was safe to be used
- Expected to be autonomous in our day to day work caring for over 120 campers a week

### Development Experience \_\_\_\_\_

#### Significant Contributions

Aug 2018 - Present

- Published cheminformatics python library "ChemScI" on github which allows conventional and custom chemical features to be easily combined with scikit-learn / machine learning pipelines.
- Three years of machine learning, python programming, and data analysis experience
- Routinely help colleagues and postgraduates with programming / data analysis queries
- During COVID-19 have gained significant experience collaborating on active code development and incorporating best practises like automated testing for continuous integration, and version control
- · Have experience working with linux environments on HPC systems

#### Other

Aug 2018 - Present

- · Have began establishing an applied machine learning interest group at University of Bath
- Member of the teaching team for University "Research software skills" courses which teach postgraduates and academics best coding and development practises
- Attended the 2019 HPC Autumn Academy at Cambridge University, a 2 week course on writing efficient and parallel C++ code for distributed systems
- Have completed Andrew NG's Machine Learning course on coursera, implementing the discussed algorithms in python using base libraries to expand my knowledge of machine learning techniques

### Other Achievements & Interests

#### **Achievements**

Ongoing

- Completed the Microsoft accredited course on "Azure Cloud Fundamentals" (2020)
- Abel & Imray prize for best research project (2019)
- Scottish Institute for Enterprise Get "Enterprising" National winner (2015)
- "Race 2 Budapest" Charity Hitchhike Logistics Officer (2015)
- University of St Andrews Jujitsu Club Treasurer & Equipment Officer (2013-2015)
- "Race 2 Berlin" charity hitchhike race from Glasgow to Berlin (2014)