

# Ferdinand George Popham Krammer | 2<sup>nd</sup> Year PhD Candidate

## University of Bath

Nationality: British, Austrian

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### Personal Profile:

I am a driven individual with a desire to learn and gain experience in new areas: to both challenge myself and further develop my skill set. I am currently in the second year of my PhD in Computational Chemistry under Dr Matthew Grayson at the University of Bath, in the Accountable, Responsible, Transparent AI Centre for Doctoral Training (CDT). Through my PhD I have sought to gain experience and develop my skills in new and emerging areas of Computational Chemistry, with a particular focus on how different Machine Learning (ML) algorithms and strategies can be used.

### Skills

- Machine learning with Python (experienced using PyTorch, TensorFlow, PyTorch Geometric, and scikit-learn)
- Data manipulation and visualization with Python, MATLAB and Excel
- Experience with High Performance Compute (University of Bath Anatra and Hex)
- Experience with Job Scheduling Software (Slurm, HTCondor, task-spooler).
- Computational modelling software (Gaussian, Orca, Schrödinger-Maestro, Schrödinger-MacroModel)
- Version control with Git and GitHub
- Regular use of different operating systems (Windows and Linux)
- Languages: English (native), German (conversationally fluent, writing at an advanced level – taken University courses up to Level 6 while at Imperial College London (comparable to C2))
- First Aid (16-hour course)

### Education

**University of Bath – PhD and MRes, in Accountable, Responsible, Transparent AI    2021 – present**

**MRes (Awarded upon completion of the PhD)**

**2021 – 2022**

As part of the CDT for Accountable, Responsible, Transparent AI (art-ai), I have been required to undertake a mandatory period of training, this takes the form of a Master's which is awarded upon completion of the PhD. As part of Master's year, I took modules in Engineering, Social Science and Computers Science focusing on Artificial Intelligence (AI) and Machine Learning. This gave me a good grounding in the theoretical and the practical implementation of ML models, gaining experience in more traditional ML techniques as well Deep Learning, working both collaboratively as part of interdisciplinary teams as well as individually on projects.

**PhD**

**2022 – present**

Since transferring from the MRes year to the PhD along with carrying out my research, I have continued to solidify my knowledge in both ML and Computational Chemistry by tutoring first and second year students in both fields, in the Computer Science and Chemistry Departments, for the last two years. I have also sought to further my knowledge of different aspects of ML by auditing a range of different ML courses such as Natural Language Processing and Reinforcement Learning.

**Imperial College London – MSc in Chemistry with Molecular Physics (1<sup>st</sup> Class)    2017 – 2021**

I achieved a First-Class Honours Degree, during which I undertook modules in Organic, Inorganic and Physical Chemistry as well as Maths and Physics courses. Through my degree I developed a keen interest in both Organic and Physical Chemistry taking, modules such as:

- Advanced Synthesis
- Reactive Intermediate Synthesis

- Plastic Electronics
- Renewable Energy

- Interfacial Science

My final year project was in “*Electrochemical Photonics: Theory of Electrotuneable Optical Metamaterials*” under Prof. Alexei Kornyshev.

## Research Experience:

### University of Bath – PhD:

**2022 – present**

In my PhD, I have used a range of different computational techniques to understand and predict chemical reactivity, to aid with the drug development process. To do this I have used molecular modelling, as well as a range of different ML techniques, to design and train different models to predict on both proprietary and publicly available datasets. Recent projects of mine have utilised the graphical nature of chemistry to design custom geometric deep learning models as well as using active learning to predict a reaction’s reactivity. This has allowed me to explore new areas of ML, whilst also allowing me to strengthen my coding and understanding of different modelling techniques. My PhD is being carried out in collaboration with AstraZeneca.

### Imperial College London – MSc Research project:

**2020 – 2021**

My fourth-year Master’s project, carried out under the supervision of Prof. Alexi Kornyshev, examined how reflection and transmission spectra changed with the adsorption of nanoparticles on different hyperbolic meta-materials. This work has been published in *Nanoscale Horizons*. In this project I developed the mathematical theory which describes the interaction of light with the nanoparticles adsorbed on hyperbolic metamaterials. I then implemented the maths in MATLAB, so that the resulting spectra could be compared to those generated through physical modelling. This project developed my interest in coding, as well as my desire to understand and be able to predict the fundamental principles governing our surroundings.

### Imperial Collage London - Undergraduate Research Opportunities Project (UROP): Summer 2019

I undertook a summer research project at Imperial College London in the Chemistry Department under the supervision of Prof. Don Craig. In this project I was synthesising novel molecules from L-leucine via 1,2,3,4-tetrahydropyridines, exploring the reactivity of these compounds. As this project was lab based it gave me an appreciation of how experiments don’t always yield the expected results. This led me to develop an interest in how reaction outcomes can be predicted via computational methods.

## Publications and Presentation history:

- PhD work:
  - **Best 1<sup>st</sup> year Computational Poster** – Boland Symposium, University of Bath 2023
  - Poster presentation – ICAS Symposium, University of Bath, 2023
  - Poster presentation – Foundational AI CDT Hackathon, 2023
- Master’s project:
  - Zagar, C., **Krammer, F.G.**, Pendry, J.B. and Kornyshev, A.A., 2022. Optical response of hyperbolic metamaterials with adsorbed nanoparticle arrays. *Nanoscale Horizons*, 7(10), pp.1228-1239.

## Personal Interests:

Much of my spare time is either spent in the hills - climbing and mountaineering, both in the summer and winter; or else kayaking – playing competitive canoe polo, as well as teaching new paddlers. Part of my enjoyment of these sports is due to the complex challenges they present, with solutions needing to be specific to the problem encountered and requiring planning and constant re-evaluation to avoid dangerous situations developing. I believe I thrive in these situations due to my methodical approach, good communication skills, and my ability to work well in a team where each member’s skills are valued and utilised.

## References provided upon request