Dr. Alexander van Teijlingen

Currently living in Glasgow

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github.com/avanteijlingen

Scientific interests

- Machine learning
- Molecular dynamics
- Reaction mechanisms
- Self-directed active learning algorithms

Education

2022. **PhD in Computational Chemistry**
University of Strathclyde
Glasgow – Scotland

2019. **MSc in Nanomaterials**
Distinction
University of Bristol
Bristol – England

2018. **BSc in Chemistry**
First Class Honours
University of Bangor
Bangor – Wales

Current Position

October 2022 – Current **Research Associate (University of Strathclyde)**

I am currently using machine learning techniques to accelerate the discovery of novel pore-forming peptides. I am also using deep learning neural network methods to screen catalytic chemical space for new catalysts with enhanced activity and to elucidate their associated reaction mechanisms.

Highlighted Skills

scikit learn PyTorch FAST. FLEXIBLE. FREE. GROMACS

Awards

Early Career Invited Presentation Award (Materials Research Society, 2023, San Francisco)

Best Research Poster Award (Peptide Self-Assembly Conference, 2023, Manchester)

Experience

July 2017 – August 2017 **Siemens Healthineers (Internship)**

Verifying the accuracy of blood test kit batches to different national standards. Writing scripts to automate analytical verification processes.

August 2014 – August 2015 **H2-ecO (Coordinator of IT)**

Maintaining customer databases, the company website and email system.

Highlighted Publications

van Teijlingen, A.; Tuttle, T. Beyond Tripeptides Two-Step Active Machine Learning for Very Large Data Sets. *J. Chem. Theory Comput.* 2021, doi: 10.1021/acs.jctc.1c00159

van Teijlingen, A. *et al.* Constant pH Coarse-Grained Molecular Dynamics with Stochastic Charge Neutralization. *J. Phys. Chem. Lett.* 2022, doi: 10.1021/acs.jpclett.2c00544