Dr Max Winokan

Computational Chemistry & Physics

Nationalities: German & American, Languages: English, German, Dutch, and Russian

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Experience

Diamond Light Source, Didcot / University of Oxford **Jul. 2023 –**

PDRA – Antiviral Computational Chemistry

- Compound design and experiment selection for high-throughput SAR on fragments
- Development and implementation of HIPPO, a Python package to make interaction-informed sampling decisions that honour experimental data for fragment progression
- Development of Python tools for drug discovery MolParse and PoseButcher
- Project and contractor management for the Fragalysis structural dissemination cloud
- Presentation of the XChem facility, ASAP project, and HIPPO & Fragalysis tools at events

University of Surrey, Guildford **Jan. 2020 – Dec. 2023**

PhD Researcher

- Developed MolParse for parsing, manipulating and analysing molecular simulation
- Applied and developed cutting edge quantum-classical (QM/MM) modelling techniques to proton transfer in large protein-DNA-solvent complexes
- Reaction mapping through steered multiscale molecular dynamics and nudged elastic band methods. Free energy analysis and quantum tunnelling corrections
- Benchmarking and optimisation of parallel simulation procedures for efficient HPC use
- Development of tools for intuitive and efficient management of HPC simulation jobs

Electronic Arts, Guildford **Jul. 2021 – Jan. 2022**

Software Engineer, Intern

- Worked in the character physics team to improve the character creation workflow,
- Overhauled a Python/PyQT GUI tool for the semi-automatic creation of character ragdolls in the Frostbite Maya pipeline. Created an intuitive interface to joint and volume creation algorithms. Produced written and video documentation
- Rebuilt a system of C++ classes to use an updated physics framework for seamless simulation of physics scenes in Maya, and in a proprietary visual debugger

TRIUMF, Vancouver, Canada **Feb. 2018 – Dec. 2018**

Graduate Research Assistant

- Worked with data acquisition systems, cryogenics, HPGe detectors, radiation sources.
- Developed and ran Geant4 simulations, built and applied numerical methods in C++
- Designed, simulated, tested, and produced SiPM readout and amplifier electronics
- Developed 3D models for visualisation, simulation and for prototyping (3D printing)

Education

University of Surrey **Jan. 2020 – Jul. 2024**

PhD Computational Physics / Chemistry. Thesis: "Multiscale modelling of DNA point mutations: the effect of the environment and replication enzymes"

University of Surrey **Oct. 2015 – Jul. 2019**

MPhys Physics: 1st class honours master's degree with a research dissertation. Average: 80%

British School of Amsterdam

A Level	Physics (A*), Mathematics (A), Biology (A), German (A*)	**2015**
AS Level	English Language and Literature (B)	**2014**
GCSE	14 Subjects (10 A* / 4 A grades)	**2013**

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Key Skills and Interests

Drug Discovery

Real-world experience on academic and industrial fragment-based drug discovery campaigns carried out at Diamond Light Source. Developed computational tools for fragment progression (hit-to-lead), aided in structural data analysis and dissemination, and compound procurement.

Project Management

Managed compound design, review, and ordering for target enablement projects in ASAP and READDI. Managed contracted software engineers for the developmend of the Fragalysis cloud.

Computational Chemistry

Excellent experience and understanding of methods fundamental to computational chemistry. Software experience: Gromacs, Amber, NWChem, RDKit, PyMOL, CP2k, CASTEP, ASE, VMD, SAMSON.

- Molecular Dynamics • Ligand Parametrisation • Force Field Generation
- Quantum Chemistry • Reaction Mapping • Proton Transfer • QM/MM
- Density Functional Theory • Nudged Elastic Band • Umbrella Sampling
- Steered MD • Topology Generation • Sequence Mutations • Annealing

Software Engineering

Proven software engineering and development skills in several languages with a passion for creating user-friendly tools and efficient algorithms. Most proficient in Python, C++, FORTRAN, BASH, SQL, HTML & JavaScript.

- Object-oriented programming • High precision numerical methods
- Numerical calculus • Differential equations • Monte-carlo methods
- Neural networks, genetic algorithms, pathfinding, computer vision
- Parallel Programming MPI & OpenMP • FFT • Linear Algebra (LAPACK)
- BASH Scripting • UNIX System Administration • HPCs • SLURM
- Version Control (git & perforce) • Large C++ projects • Makefiles
- Interface Design • PyQt • Tk • HTML/CSS/JS • Visualisation & animation

Experimental

Practical experience during my Master's research, resulting in a thorough understanding of experimental uncertainty and associated data analysis.

- Radiation detectors • Electronic design/prototyping • Signal processing
- Optical and nuclear spectroscopy • Nuclear magnetic resonance
- X-ray diffraction • Cryogenics • Radioactive sources • Vacuum systems

Scientific Communication

I have published four peer-reviewed publications as 1st or 2nd author and have presented award-winning posters and presentations at scientific conferences.

Visual

Long-term interests in photography, 3D modelling/animation, and graphic design. Highly skilled in Adobe Photoshop and Illustrator. Experienced in creating beautiful 3D renders of chemical systems.

Referees

Prof. Frank von Delft
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Dr Warren Thompson
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