max@winokan.com
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Dr Max Winokan

Computational Chemistry & Physics

Nationalities: German & American, Languages: English, German, Dutch, and Russian
winokan.com

Experience

Diamond Light Source, Didcot **Jul. 2023 –**
PDRA – Antiviral Computational Chemistry

AI-driven Structure-enabled Antiviral Platform (ASAP) Consortium

- Coordination of the compound design for the target enablement projects at XChem.
- Development and implementation of HIPPO, a Python package to make interaction-informed sampling decisions that honour experimental data for follow-up selection
- Steering contracted engineers to improve the frontend interface of the Fragalysis cloud
- Development of graphical and analytical tools for the Fragalysis cloud platform
- Presentation of the XChem facility, ASAP project, and HIPPO & Fragalysis tools at events

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

Multiscale modelling of DNA point mutations:
the effect of the environment and replication enzymes

- 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 **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

Computational Chemistry

Excellent experience and understanding of methods fundamental to computational chemistry. Software experience: Gromacs, Amber, NWChem, RDKit, CP2k, CASTEP, ASE, VMD, SAMSON. I have developed a python library for working with molecular structure files, interfacing to chemistry software, and data analysis named MolParse.

Experience with:
• 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, and BASH with working knowledge of HTML and JavaScript.

Experienced in:
• 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

Hundreds of hours of practical laboratory hours and several days of experimental shifts during both my masters research, resulting in experimental experience and a thorough understanding of experimental uncertainty, and associated data analysis.

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

Communication

Excellent experience in oral presentations, debating, and poster presentation at scientific conferences. Good skills in writing proven through published scientific articles and master's dissertation.

Visual

Long-term personal 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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