

Jeremy Rabone - CV

Professional Experience

- Apr. 2008 **Research Associate**, *Chemistry department, Liverpool University.*
- Simulation of Metal Organic Frameworks to steer laboratory investigations
 - Molecular dynamics simulations using DLPOLY on NW-GRID and NGS clusters
 - Structure prediction to assist elucidation of novel structures
 - DFT calculations using VASP to complement the atomistic simulations.
 - High-throughput screening of enantiomers with chiral frameworks
 - Development of Java tools to handle and validate chemical structure databases
 - Docking of enantiomers with chiral frameworks using AutoDock
- Jan. 2003 –
Dec. 2004 **Freelance Computational Chemist / Programmer**
- Unilever NV*
- Software development (C++ and Java), including chemical simulation and visualisation tools, 3D modelling (molecule representations) and animation
- Four Delta Consulting Ltd*
- Scientific / corporate website development
- Evotec OAI, Hamburg – EC Leonardo Programme support*
- Installation / optimisation of ISIS Host 5.0 and Oracle 9i for pharmaceutical database
 - Normalisation of structures in 750,000 chemical compounds database using Java
 - Methods for database validation, identifying identical structures, and database-processing
 - Exposed to high-throughput methods in drug discovery
- Sep. 2000 –
Dec. 2002 **Research Associate**, *Unilever R&D Laboratory, Port Sunlight*
- Chemical simulation [food flavours] software and databases (C++) with support programs in Java
- Special achievement:** Two patents filed, based on the flavour generation (Maillard Reaction) computer tool developed.
- Statistical analysis tools for large consumer datasets (numerical and textual data) (Java / Matlab)
 - Text-mining tools (Java / Perl) for Competitive Technical Intelligence and Consumer Relationship Management
 - Demonstration systems for knowledge representation languages – artificial reasoning for consumer dialogue (Java / XML)
- Special achievement:** Best paper/poster prize at Corporate Review May 2003.
- Game concept demonstrations, short multimedia scenarios and mock up Web site for on line consumer interaction and consumer – avatar dialogue (Visual C++ / HTML / JavaScript / XML)
 - Technical support, maintenance and training of a digital media laboratory for Business Science
- 1997-2000 **Intern (university holidays)**, *Unilever R&D Laboratory, Port Sunlight*
- Chemical simulation software to aid the analysis of complex systems of chemical reactions (C / C++)
- Initial chemical reaction databases with a team of organic chemists to apply the simulation software above to reactions occurring in food preparation (Maillard Reaction)

Education and Qualifications

- Jan. 2005 – **PhD**
Dec. 2007 University & Birkbeck Colleges, University of London
- Apr. 2006 – **Support Technician** (Materials Molecular Dynamics Network)
May 2006 University of Limpopo, South Africa
- Jul. 2005 **Collaborative Computational Projects 5**
Marie Curie Actions Molecular Simulation Summer School
Cardiff University
- Apr. 2005 **X-Rays, Neutrons and Computers in Materials Chemistry**
Mansfield College, Oxford
- Sep. 1996 – **M. Chem. (2.i)**
Jun. 2000 Worcester College, University of Oxford
- Master's Thesis:** "Surfactant – Clay Interactions"
Investigation, using X-Ray diffraction, of a synthetic route to pillared clays via surfactant intercalation
- Special achievement:** Awarded a University scholarship for outstanding performance in first year's examinations.
- Sep. 1989 – **A1 (Chemistry), A (Physics, Maths, Further Maths, Geology, Gen. Studies)**
Jun. 1996 Wirral Grammar School for Boys
- Special achievements:**
- Represented the U.K. in the 28th International Chemistry Olympiad (Moscow, 1996). Individual bronze medal; joint 8th out of 42 countries as part of UK team.
 - National Geology prize for best candidate.

Additional Information

- British National
- References available on request