

# Herbert Früchtl

## EaStCHEM Fellow

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Research Interests: Computational Chemistry



My role is to manage the St Andrews branch of the EaStCHEM Research Computing Facility. All questions regarding access to the facility, problems with hardware or software, as well as requests for software to be installed should be directed to me.

I advise on all matters connected to computational simulation. My remit involves finding out which chemical or physical properties can be determined through numerical simulation, which software to use and what accuracy can be expected. I collaborate with various research groups, complementing their experimental research with computational studies.

### SELECTED PUBLICATIONS

T. van Mourik and H.A. Früchtl, "The Potential Energy Landscape of Noradrenaline. An Electronic Structure Study", *Mol. Phys.* **103**, 1641-1654 (2005).

R.A. Kendall and H.A. Früchtl, "The impact of the Resolution of the Identity (RI) approximate integral method on modern ab initio algorithm development", *Theor. Chem. Acc.* **97**, 158 (1997).

R.H. Nobes, H.A. Früchtl and E.V. Akhmatskaya, Parallel MOZYME, *Proc. Third High Performance Computing Asia Conference*, 753 (1998).

A.P. Rendell, A. Bliznyuk, T. Huber, R.H. Nobes, E.V. Akhmatskaya, H.A. Früchtl, P.W.-C. Kung, V. Milman and H. Lung, "Computational Chemistry on Fujitsu Vector-Parallel Processors: Development and Applications Software", *Parallel Computing* **26**, 887 (2000).

H.A. Früchtl, R.H. Nobes and A. Bliznyuk, "Performance of MOPAC on Parallel Computers", *THEOCHEM* 506, 87 (2000).

M. F. Guest, E. Apra, D. E. Bernholdt, H. A. Fruchtl, R. J. Harrison, R. A. Kendall, R. A. Kutteh, X. Long, J. B. Nicholas, J. A. Nichols, H. L. Taylor, A. T. Wong, G. I. Fann, R. J. Littlefield and J. Nieplocha, "High-Performance Computing in Chemistry; NWChem", *Future Generations Computer Systems* **12(4)**, 273, (1996).