

UniCat Colloquium

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- Lecturer: **Prof. Robert J. Deeth**, Computational Chemistry, Department of Chemistry, University of Warwick, Coventry, UK
- Title: **Computational Coordination Chemistry and DFT: Time for Force Fields to Make a Comeback?**
- Abstract: Density functional theory (DFT) has revolutionised our ability to perform relatively accurate quantum chemical calculations on transition metal (TM) systems in a reasonably short time. Yet, even during the 1990's as the revolution gained momentum, it was clear that no quantum method would ever be able to compete with the raw speed of classical molecular mechanics (MM). The problem is that MM is not well suited to TM systems. "Conventional" MM cannot handle in a general way the all-important d-electron stereoelectronic effects characteristic of many TM systems. MM thus presented little competition to DFT. However, 40 years of applying ligand field theory (LFT) to TM complexes had shown that the special features of TM systems could be explained by an empirical model. Thus, we began a program to exploit the extensive LFT knowledge base to construct an augmented form of MM specifically designed for open shell transition metal systems with all their attendant structural and electronic properties. This talk will describe the development of our new 'classical' model: ligand field molecular mechanics (LFMM). LFMM can be parameterised to reproduce DFT and/or experiment to high accuracy but runs at least four orders of magnitude faster. LFMM thus can access virtual high-throughput screening, comprehensive conformational searching and molecular dynamics simulations which are simply too expensive for DFT. Here, I will outline the strengths and weaknesses of LFMM together with past, present and future applications in coordination and bioinorganic chemistry.
- Find more about Prof. Deeth on:
<http://www2.warwick.ac.uk/fac/sci/chemistry/research/deeth/deethgroup>
- Date: **Wednesday, November 13th, 2013 at 5:15 pm**
- Location: **TU Berlin, Department of Chemistry
Straße des 17. Juni 115, 10623 Berlin
Building C, Lecture Hall C 264**
- Organiser: **Prof. Martin Kaupp (TUB)**

Coffee and tea will be served thirty minutes prior to the lecture start.
Guests are cordially invited to attend!

Prof. Dr. Matthias Driess, Chair of the Cluster of Excellence UniCat