"The Nitrogenase Challenge. Synthetic Methodology and Assembly of Homo and Hetero-nuclear M/S Clusters"

Following the original EXAFS studies on the Fe/Mo/S center in nitrogenase, and the structural information provided from these studies, attempts towards the synthesis of possible Fe/Mo/S analog clusters started in earnest. Since 1979 Coucouvanis has been developing this chemistry starting with simple \( \text{S}_2\text{MoS}_2\text{Fe} \) dimers and \( \text{FeS}_2\text{MoS}_2\text{Fe} \) trimers, obtained using the \( \text{MoS}_4^{2-} \) anion as a ligand. The stepwise synthesis of MoFeS clusters continued over the years and the fundamental chemistry of these molecules was developed with the prismane adducts, the singly and doubly bridged double cubanes, the fused double cubanes and Roussin type clusters with the \([\text{MoFeS}_3]^2+\) cores. The structures of the latter, and Density Functional Theory (DFT) calculations, suggested strong Fe-Fe attractive interactions that may also be present in the nitrogenase cofactor. Recent studies in the synthesis of heterometallic clusters have lead to the rational assembly of \( M_{8-n}M'_nS_6 \) clusters with a pentlandite core structure and \( M, M' = \text{Fe}, \text{Ni}, \text{Cu}, \text{Zn} \); \( n = 2, 3 \) and 4.

"Di- and Tetranuclear transition metal complexes with bridging ligands. Quantum chemical interpretation of spectral and redox properties."
The electronic structures of di- and tetraneuclear transition metal complexes with bridging ligands (azobypiridine, tetracyanoethene, tetracyano-p-quinodimethane and divinylphenylene) were calculated by density functional (DFT) method. DFT method was used for calculations of IR frequencies in different oxidation states and EPR parameters of radical ions. The observed electronic transitions of closed shell systems were assigned by TD DFT. The different aspects of bridge mediated metal-metal interaction will be discussed.

- **PhD John F. Corrigan**  
  Department of Chemistry, Ontario  
  Donnerstag, 22. Juni 2006  
  17.15 Uhr, H 46  
  **Gastgeber: Prof. Manfred Scheer**  

"Metal-chalcogenolate Complexes for Ternary Nanocluster and Nanoparticle Synthesis"

Coordination complexes containing the groups –ESiMe₃ (E = S, Se, Te) represent viable reagents for the controlled synthesis of ternary metal chalcogenides, M-E-M', serving as soluble sources of M-E. The chalcogen reagents, with a pendant trimethylsilyl moiety, react with metal salts, M'-X, via the elimination of Me₃SiX (X = halide, OAc, etc) and the formation of M-E'M' bonds. We have recently prepared a series of metal-chalcogenolates of the group 11 and 12 metals, LₓM-(ESiMe₃)ₙ (L = ligand; n = 1, 2) in excellent yields. Details on the preparation and properties of LₓM-(ESiMe₃)ₙ, in particular their utility in the preparation of nanometer sized ternary semiconductor clusters and particles, will be presented. Under mild conditions, luminescent ternary nanoclusters and nanoparticles (e.g. ZnₓCd₁₋ₓSe, ZnₓCd₁₋ₓTe) can be formed.

- **Prof. Ulrich Siemeling**  
  Fachbereich 18, Metallorganische Chemie, Uni Kassel  
  Donnerstag, 06. Juli 2006  
  17.15 Uhr, H 46  
  **Gastgeber: Prof. Rainer Winter**  

"Enjoying Chemistry with Functionalised Ligands: From Chelate Complexes to Functional Surfaces"

The modification of ligands by functional groups can lead to novel, emergent ligand properties. Our group has focussed on bi- and tridentate ligands which contain redox- or photo-active groups. We are investigating the interaction of such ligands with metals both in molecular coordination chemistry and in surface chemistry, where we are addressing the
fabrication and properties of functional self-assembled monolayers which are able to respond to external stimuli. In this context, a task of fundamental importance is to bridge the gap between molecular and surface chemistry. For example, in the case of 1,1'-diisocyanoferroocene (1), the crystal structure of the aurophilic polymer [(1)(AuCl)2]ν (a section is shown below) provides a model for the binding and arrangement of the 1,1'-diisocyanoferroocene adsorbate molecules on a gold surface.

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**Prof. Matthias Driess**  
Fachgruppe Anorganische und Analytische Chemie, Tu Berlin  
17.15 Uhr, H 46  
Gastgeber: Prof. Manfred Scheer

"Chemische Tricks mit schweren Elementen: Von nucleophilen Carben-Analoga zu elektrophilen Katalysatoren"


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*Rückblick der Vorträge in den vergangenen Semestern:*

- **Wintersemester 2005/2006**
- **Sommersemester 2005**
- **Wintersemester 2004/2005**
• Sommersemester 2004
• Wintersemester 2003/2004
• Sommersemester 2003
• Wintersemester 2002/2003
• Sommersemester 2002
• Wintersemester 2001/2002
• Sommersemester 2001