

## VORTRÄGE 2012

**Albers**, Antonia:

A Functional Model for Rieske-type [2Fe-2S] Clusters

*Joint Workshop IRTG 1422 und FOR 1405 in Hofgeismar, 12.04.12*

**Beer**, Günther:

Lampadius' akademisches Umfeld an der Universität Göttingen

*Vortragstagung: Wilhelm August Lampadius 8. August 1772 – 13. April 1842 Chemiker, Erfinder, Fachschriftsteller und Hüttenmann, Freiberg (Sachsen), 11.-14.04.12*

**Böhnisch**, Torben:

C<sub>2</sub>-Symmetric Pyrazolate-Bridged Bis(oxazoline) Ligands: New Scaffolds for Bimetallic Asymmetric Catalysis

*Joint Workshop CaSuS/NanoKat, Braunfels, 28.06.12*

**Burger**, Boris:

The Carboxylate Shift and the Carboxylate Twist: Unusual Dynamics at Pyrazolate-based Bioinspired Diiron Sites

*8. Koordinationschemie-Treffen, Universität Dortmund, 26.-28.02.12*

**Carl**, Elena:

Metal Complexes of Polyimido Phosphanyl Sulfur Ligands

*CaSuS Tagung, Wetzlar, 27.-29.06.12*

**Clever**, Guido H.:

Beyond Platonic Solids: Low Symmetric, Intertwined and Interpenetrated Coordination Cages

*Inorganic Chemistry Colloquium, RWTH Aachen, 20.01.12*

**Clever**, Guido H.:

Control over Cavity Size & Shape in Anion-binding Coordination Cages

*Chemistry Colloquium, Jacobs University Bremen, 13.12.12*

**Clever**, Guido H.:

Coordination Cages

*BuilMoNa Graduate School workshop, Leipzig University, 27.-29.06.12*

**Clever**, Guido H.:

Functional Coordination Cages: Structural Complexity, Guest Binding and Impulses for Energy Conversion Processes

*Second German-Japanese University Presidents' Conference HeKKSaGOn, Kyoto University, 29.-30.03.12*

**Clever**, Guido H.:

Functional Coordination Cages: Structural Control, Metal Stacking and Allosteric Ion Binding

a) *Fudan University (Shanghai), 23.04.12*

b) *East China Normal University (Shanghai), 24.04.12*

c) *Zhejiang University (Hangzhou), 25.04.12*

d) *Nanjing University (Nanjing), 02.05.12*

e) *Nanjing University of Technology (Nanjing), 03.05.12*

f) *Alexander von Humboldt Foundation's 5th Sino-German Frontiers of Science (SinoGFOS) symposium, Nanjing, China, 26.-29.04.12.*

**Clever**, Guido H.:

Interpenetration und allosterische Anionenbindung von Supramolekularen Koordinationskäfigen

*Chemiedozententagung Freiburg, 04.-06.03.12*

**Clever**, Guido H.:

Positive Cooperativity in Anion Binding by Light-switchable and Interpenetrated Coordination Cages

*SFB 858 (Cooperative Effects) workshop, Münster University, 14.08.12*

**Clever**, Guido H.:

Structure-Function Relationships in Coordination Cages

*International Conference on Coordination Chemistry (ICCC), Valencia, 09.-14.09.12*

**Clever**, Guido H.:

Structure-Function Relationships in Anion-Binding Coordination Cages

*Inorganic Chemistry Colloquium, Köln University, 05.12.12*

**Clever**, Guido H.:

Switchable and Allosteric Anion Binding in Self-Assembled Coordination Cages

*Japanese-German Symposium on Coordination Programming, Münster University, 25.-27.20.12* □

**Clever**, Guido H.:

Verheddert, gestaucht und verknotet: Koordinationskäfige jenseits Platonischer Körper

*Chemistry Colloquium, TU Braunschweig, 09.05.12*

**Dauer**, David-Raphael:

On the brink to metallocarbenes

*Center for Materials Crystallography (CMC) 5<sup>th</sup> workshop, Aarhus/DK, 14.08.12*

**Dittrich**, Birger ; **Hübschle**, Christian B.:

Introduction to MolecoolQt

*The 27th European Crystallographic Meeting, Bergen, Norway, 07.08.12*

**Dittrich**, Birger ; **Pröpper**, Kevin ; **Meents**, Alke ; **Bond**, Charles S.:

On combining synchrotron radiation and invariom refinement: opportunities for high-throughput small molecule and ultra-high resolution macromolecular refinement

*SAGAMORE XVII Conference on Electron Charge, Spin and Momentum Densities, Hokkaido (Japan), 15.-20.07.12*

**Dittrich**, Birger:

Non-spherical electron densities using invarioms: Introduction, applications and examples of invariom refinement

*Bruker webinar, 08.05.12*

**Engelhard**, David:

NMR-Based Structure Determination of an Intertwined Coordination Cage resembling a Double Trefoil Knot

*Göttinger Chemie Forum 2012, Göttingen, 11.07.12*

**Engelhardt**, Felix:

Charge Density Distribution in [(diglyme)<sub>2</sub>Li][Cp<sub>2</sub>Li]

*CMC 6<sup>th</sup> workshop, Göttingen, 22.11.12*

**Frank**, Marina:

Funktionelle multitone und dendritische Organisationseinheiten auf Basis von Koordinationskäfigen und deren Aggregation zu redoxaktiven Vesikeln und Oberflächen

*Evonik Foundation meeting, Essen, 03.05.12*

**Freye**, Sabrina:

Allsterische Halogenidbindung durch einen interpenetrerenden Doppelkäfig

*Koordinationschemietreffen Dortmund, 28.02.12*

**Ghadwal**, Rajendra:

Kleine, aber ungewöhnliche Moleküle

*GDCh Weihnachtskolloquium der Fakultät für Chemie, Göttingen, 13.12.12*

**Granitzka**, Markus:

[2-Thienyllithium\*diglyme] - a Pentuple Ion

*Center for Materials Crystallography (CMC) 5<sup>th</sup> workshop, Aarhus, DK, 13.8.12*

**Granitzka**, Markus:

Single Crystal, Split or Powder - Criteria of Data Quality

*APEX2 Workshop – Twinning and Disordered Samples, Taipeh (Taiwan), 20.03.12*

**Grüne**, Tim:

1) Advanced Applications of SHELXD and SHELXE

2) Macromolecular Phasing: Solving the Substructure

*Present and Future Methods for Biomolecular Crystallography", Erice, Italien, 5.-6.06.12*

**Grüne**, Tim:

- 1) The Shelx Suite: Applications to Macromolecular Crystallography
  - 2) Fundamentals on Diffraction Data Integration and Data Reduction
- Macromolecular Crystallography School", Madrid, Spanien, 26.-27.05.12*

**Grüne**, Tim:

How to trace polynucleotides  
*20th Bruker Users' Meeting, Bad Herrenalb, 27.09.12*

**Grüne**, Tim:

Macromolecular Phasing with SHELX C/D/E  
*CCP4/APS Summer School", Chicago USA, 22.06.12*

**Grüne**, Tim:

Refinement of Macromolecular Neutron Data with shelxl  
*BER-II Users' Meeting, Berlin, 12.12.12*

**Guo**, Tongxun:

Pyrazole-Bridged Bis-(N-Heterocyclic Carbene)Ligands and their Bimetallic Palladium Complexes  
*Joint Workshop CaSuS/NanoKat, Braunfels, 27.06.12*

**Han**, Muxin:

Controlled Self-Assembly of Coordination Cages through Rational Ligand Design  
*15. Norddeutsches Doktorandenkolloquium, Krelingen, 24.09.12*

**Han**, Muxin:

Self-Assembled Coordination Cages and Their Structural Control by Subtle Ligand Variation  
*Joint Workshop CaSuS/NanoKat, Braunfels, 27.06.12*

**Herbst-Irmer**, Regine

Anharmonic Nuclear Motion in Charge Density Studies  
*10 Years Incoatec, Workshop on Instrumentation & Science, Geesthacht, 01.06.12*

**Herbst-Irmer**, Regine:

- 1) Constraints and Restraints
  - 2) Introduction to Twinning
  - 3) Examples of (Pseudo-)Merohedral Twins
  - 4) Examples of Twinned Structures: Non-merohedral Twins
- Bruker Workshop on Problem Structures, Taipei, 20.-22.03.12*

**Herbst-Irmer**, Regine:

Anharmonic Motion in Charge Density Studies  
a) *6<sup>th</sup> European Charge Density Meeting, Strbske Pleso, 15.-20.09.12*  
b) *CMC, 6<sup>th</sup> Workshop, Göttingen, 22.11.12*

**Herbst-Irmer**, Regine:

Resolution dependent scaling – a solution for problems in a multipole refinement  
*27<sup>th</sup> European Crystallographic Meeting, Bergen, 06.-11.08.12*

**Hey**, Jakob:

A Crystallographic Study on a Very Small Piano Stool Complex  
*CMC 6<sup>th</sup> workshop, Göttingen, 22.11.12*

**Hey**, Jakob:

Demonstration Lesson on Disorder  
*APEX2 Workshop – Twinning and Disordered Samples, Taipeh (Taiwan), 20.03.12*

**Hübschle**, Christian B. ; **Dittrich**, Birger ; **Sheldrick**, George M.:

ShelXle - A cute GUI for SHELXL  
*20th Annual Meeting of the German Crystallographic Society (DGK) Munich, 13.03.12*

**Hübschle**, Christian B. ; **Dittrich**, Birger ; **Sheldrick**, George M.:

ShelXle a graphical-user-interface for SHELXL  
*20th users' meeting in Single Crystal X-ray Diffraction in Bad Herrenalb, Germany, 24.09.2012*

**Hübschle**, Christian B.:

New Features in MoleCoolQt

*European Charge Density Meeting – ECDM6, Strbske Pleso, Slowakia, 19.09.12*

**Irmer**, Erhard ; **Wolf**, Kai ; Wilke, Timm ; **Waitz**, Thomas:

Von chemischen Chamäleons und magnetisierbaren Salzen – Neues aus der Komplexchemie  
*MNU-Tagung Bremerhaven, 20. 11.12*

**John**, Michael:

$^7\text{Li}$  Residual Quadrupolar Couplings and Diffusion of Organolithiums into PS Gels

*34. Tagung der GdCh-Fachgruppe Magnetische Resonanzspektroskopie, Halle, Germany, 19.09.12*

**Kratzert**, Daniel:

A short introduction to Bruker-AXS SAINT and R-Latt

*APEX2 Workshop – Twinning and Disordered Samples, Taipeh (Taiwan), 20.03.12*

**Kratzert**, Daniel:

Two isomers of Hexasilabenzene in an Experimental Charge Density Study

*Seminar "Advanced Crystal Structure Analysis", Göttingen, Dezember 2012*

**Meyer**, Franc:

A Glimpse of the Joy of Coordination Chemistry: Biomimetic Metallosites, Bioinspired Catalysts, and Beyond

*A. Chakravorty Endowment Lecture auf dem NSC-14 Symposium, Trivandrum/Indien, 04.02.12*

**Meyer**, Franc:

Binuclear Complexes of the Siamese Twin Porphyrin

*40<sup>th</sup> International Conference on Coordination Chemistry – ICCC40, Valencia/Spanien, 12.09.12*

**Meyer**, Franc:

Controlling Metal Ion Cooperativity: Multistable Grid Complexes and the Siamese Twin Porphyrin

*Deutsch-Japanisches Koordinationschemie-Symposium, Universität Münster, 26.10.12*

**Meyer**, Franc:

Cooperating Metal Centers: from Metallobiosites to Magnetic Nanoswitches

*Indian Institute of Technology Bombay/Indien, 01.02.12*

**Meyer**, Franc:

Kooperierende Metallzentren in Mehrkernkomplexen: von Enzymmodellen zu magnetischen Schaltern  
*GDCh-Vortrag in der Chemischen Fakultät der Universität Rostock, 12.01.12*

**Meyer**, Franc:

Kooperierende Metallzentren in Mehrkernkomplexen: von Enzymmodellen zur bioinspirierten Katalyse  
*GDCh-Vortrag in der Chemischen Fakultät der Universität Regensburg, 02.07.12*

**Meyer**, Franc:

Mehrkernkomplexe als molekulare Nanoschalter

*Institutskolloquium der Universität Augsburg, 11.06.12*

**Meyer**, Franc:

Metallzentren im Duett: von Enzymmodellen zu Nanoschaltern

a) *Anorganisch- und Analytisch-Chemisches Kolloquium der Universität Marburg, 09.01.12*

b) *GDCh-Vortrag in der Chemischen Fakultät der Universität Köln, 30.10.12*

**Meyer**, Franc:

Molecular Nanoswitches – A Chemist's Approach

*Spring Workshop der NTH School for Contacts in Nanoswitches, Goslar, 11.05.12*

**Meyer**, Franc:

Neues zu biomimetischen Fe/S-Clustern, den Vielzweck-Funktionseinheiten der Natur

a) *Kolloquium der Heidelberger Chemischen Gesellschaft der Universität Heidelberg, 17.07.12*

b) *Vortrag zur Verleihung des Horst-Dietrich-Hardt-Preises, Universität des Saarlandes in Saarbrücken, 29.10.12*

**Meyer**, Franc:

New Turns in Biomimetic Fe/S Chemistry: Functional Models for the Rieske Center and Related [2Fe-2S]-Cluster

*H<sub>2</sub>-Designcells Meeting des BMBF, Köln, 04.06.12*

**Meyer, Franc:**

New Turns in Biomimetic Fe/S Chemistry: Reduced and Superreduced [2Fe-2S] Clusters and Proton-Coupled Electron Transfer of the First Functional Models for Rieske Centers  
*11<sup>th</sup> European Biological Inorganic Chemistry Conference, Granada/Spanien, 15.09.12*

**Neudeck, Sven:**

Synthesis and Investigation of New Ruthenium-Based Complexes as Water-Oxidation Catalysts  
*Joint Workshop CaSuS/NanoKat, Braunfels, 28.06.12*

**Pereira, Fernanda A.:**

Controlled folding and conformational changes in dynamics, metal-mediated DNA constructs  
*AUGM (Asociación de Universidades del Grupo Montevideo), Curitiba-PR, Brasil, 05.10.12*

**Pöppler, Ann-Christin:**

Anisotrope NMR-Spektroskopie an organometallischen Verbindungen  
*Hannover, Winterfeldtpreis 2012, Juli 2012*

**Pöppler, Ann-Christin:**

Polymer Gels for the Analysis of Organometallic Compounds in Solution  
*Second DFG research unit meeting "FOR 934", Darmstadt, 04.-05.12.12*

**Pöppler, Ann-Christin:**

RQCs - Anisotropic NMR parameters and the aggregation of lithiumorganic compounds  
*Aarhus, DK Center for Materials Crystallography (CMC) 4<sup>th</sup> workshop, 25.01.12*

**Pröpper, Kevin ; Holstein, Julian J. ; Hübschle, Christian B. ; Bond, Charles S. ; Dittrich, Birger:**  
Invariom refinement of a new dimeric monoclinic solvate of thiostrepton at high resolution.  
*IBMB-CSIC Biomed Seminar, Barcelona, 03/2012*

**Pröpper, Kevin ; Meindl, Kathrin ; Rodriguez, Dayté ; Sammito, Massimo ; Dittrich, Birger ; Sheldrick, George M. ; Pohl, Ehmke ; Usón, Isabel:**  
DNA - Protein complex structure solution.  
*30th European Crystallographic Meeting, Bergen (Norwegen), 06.-10.08.12*

**Rittmeier, Markus:**

Copper(I)-specific Chelators for the Treatment of Alzheimer's Disease  
*Joint Workshop IRTG 1422 and FOR 1405, Hofgeismar, 12.04.12*

**Roesky, Herbert W.:**

The stabilization of compounds with low valent elements in the presence of Lewis acids and bases  
*Indian International Symposium on Fluorine Chemistry, Delhi, Indien 21.02.12*

**Roesky, Herbert W.:**

Chemistry inspired by interstellar molecules  
*Annual Chemistry Lecture Nehru Center, Bangalore, Indien, 23.02.12*

**Roesky, Herbert W.:**

The impact of Bartlett's discovery on science and education  
*Bartlett Symposium 50 years of Xenon chemistry, Vancouver, Canada, 23.03.12*

**Roesky, Herbert W.:**

Fluorine compounds with low valent main group elements  
*20<sup>th</sup> International Symposium on Fluorine Chemistry, Kyoto, Japan, 23.07.12*

**Roesky, Herbert W.:**

Chemistry of low valent silicon  
a) XXV International Conference on Organometallic Chemistry, Lissabon, Portugal, 03.09.12  
b) Universität Graz, Oesterreich, 23.11.12

**Roesky, Herbert W.:**

Chemie von ihrer schönsten Seite  
*Jahrestagung der Gesellschaft der Naturforscher und Ärzte, Göttingen, 15.09.12*

**Schneider, Sven:**

Late Transition Metal PNP Pincer Platforms for Nitrogen Fixation Model Chemistry  
*XXV Internat. Conf. on Organomet. Chemistry (XXV ICOMC), Lissabon, Portugal, 02.-07.09.12*

**Sheldrick, George M.:**

A new approach to crystal structure solution  
*San Diego, USA, 23.03.12*

**Sheldrick, George M.:**  
Basic concepts of experimental phasing and substructures  
*Zaragoza, Spain, 13.03.12*

**Sheldrick, George M.:**  
Density modification and phasing with SHELXC/D/E  
*Zaragoza, Spain, 14.03.12*

**Sheldrick, George M.:**  
Progress in macromolecular phasing using in-house data  
*Bad Herrenalb, Germany, 27.09.12*

**Sheldrick, George M.:**  
SAD, SIRAS and MAD phasing with SHELXC/D/E  
*Oulu, Finland, 31.01.12*

**Sheldrick, George M.:**  
SHELXL-2012 – New ideas in crystal structure refinement  
*Bad Herrenalb, Germany, 25.09.12*

**Sheldrick, George M.:**  
SHELXL-2012.  
*ACA Meeting, Boston USA, 01.08.12*

**Sheldrick, George M.:**  
XPREP, SADABS and TWINABS  
*Oulu, Finland, 01.02.12*

**Stalke, Dietmar:**  
A World of Difference – Alkali Metal Organic Frameworks from Ammonia  
*Invited lecture at the Indo-German Conference on Complex Chemical Systems at the IISER Bhopal, India; 03.-06.12.12*

**Stalke, Dietmar:**  
Die Struktur-Reaktivitäts-Beziehung im Lichte der Dichte  
*GDCh Kolloquium an der Technischen Universität Kaiserslautern, 27.11.12*

**Stalke, Dietmar:**  
From IAM to AIM - What is required?  
*SHELX 2012 Workshop an der Universität Göttingen, 14.12.12*

**Stalke, Dietmar:**  
Lithium Ammoniacates with Cyclic Carbanions  
*1<sup>st</sup> Symposium on Industrial Organometallic Chemistry SIOC in Goslar, 04.-06.09.12*

**Stalke, Dietmar:**  
Low Valent Silicon  
a) 27<sup>th</sup> Meeting of the European Crystallographic Association ECM27 at Bergen University, Norway, 06.-11.08.12  
b) 6<sup>th</sup> European Charge Density Meeting ECDM6 in Strbske Pleso, High Tatras, Slovakia, 15.-20.09.12  
c) Plenary lecture at the 20<sup>th</sup> Bruker Users' Meeting in Bad Herrenalb, 23.-27.09.12

**Stalke, Dietmar:**  
Modulated lithium electrode affinity via ammonia donation  
*Second German-Japanese University Presidents' Conference HeKKSAGOn at the Kyoto University, Japan, 29.-30.03.12*

**Stalke, Dietmar:**  
Was lernt der präparative Chemiker aus der Elektronendichte?  
*Anorganisch Chemischen Kolloquiums an der Universität Essen, 16.01.12*

**Stalke, Dietmar:**  
What a synthetic chemist learns from charge density  
*Anorganisch Chemischen Kolloquium an der Universität Freiburg, 12.12.12*

**Thorn, Andrea:**  
An introduction to twinning  
*ZCAM Workshop 2012, Zaragoza, Spain, 12.03.12*

**Thorn**, Andrea:

Anisotropy in macromolecular crystal structures  
*GRC 'Diffraction methods', Lewiston MA, USA, 19.07.12*

**Thorn**, Andrea:

ANODE: anomalous and heavy-atom density calculation  
*Bruker User's Meeting, Germany, 26.09.12*

**Thorn**, Andrea:

Hellethionin D: A S-SAD story  
*HEC15, Beilngries, Germany, 29.09.12*

**Thorn**, Andrea:

SHELXC/D/E  
*CCP4 Workshop, Fukuoka, Japan, 31.10.12*

**Thorn**, Andrea:

Twinning  
a) *Meeting of the American Crystallographer's Association, Boston, USA, 28.07.12*  
b) *CCP4 Workshop, Fukuoka, Japan, 30.10.12*

**Waitz**, Thomas:

Innovative Lehr-/Lernformen und neue Inhalte für das Fach Chemie an Schule und Hochschule  
*Universität Münster, 14.11.12*

**Waitz**, Thomas:

„Nano“ – Ein Thema nur für die Forschung oder auch für den Chemieunterricht?  
*MNU-Tagung, Göttingen, 11.10.12*

**Waitz**, Thomas:

„Nano“ – Eine vernachlässigte Dimension im Chemieunterricht?  
*GDCh-Tagung, Freiburg, 14.09.12*

**Waitz**, Thomas:

Nanoporous Materials – From Synthesis Concepts to Chemical Education Aspects  
a) *Anna University, Indien, 23.08.12*  
b) *Pondicherry University, Indien, 28.08.12*  
c) *University of Madras, Chennai, Indien, 30.08.12*

**Waitz**, Thomas:

A Chemical Gallery Walk through German and Indian Supermarkets  
*Indo-German Urban Mela, Chennai, Indien, 26.08.12*

**Waitz**, Thomas:

Enhancing Chemical Education in Laboratory Using Videos and the LMS-ILIAS  
*Anna University, Indien, 23.08.12*

**Waitz**, Thomas:

Nanoporous Materials in Chemical Education  
*Biennial Conference on Chemical Education (BCCE), Pennstate University, USA, 01.08.12*

**Waitz**, Thomas:

Self-Assessment and Differentiated Exercising – A Promising Combination for Test Preparation  
*Biennial Conference on Chemical Education (BCCE), Pennstate University, USA, 31.07.12*

**Wolf**, Hilke:

Phase Transition in Paracyclophane  
*CMC 6<sup>th</sup> Workshop, Göttingen, 22.11.12*