

Proposal colloquium SPP 1178 Kloster Banz

Wednesday, February 04th, 2009

– 12:00		Arrival
12:00 – 12:10		Janssen <i>Welcome from the DFG</i>
12:10 – 12:20		Stalke, Göttingen / Scherer, Augsburg / Luger, Berlin <i>Welcome from the coordinators – Organizational remarks</i>
12:20 – 12:50		Stalke, Göttingen <i>Coordination and instrumentation of the SPP 1178</i>
12:50 – 14:00		Lunch
Chair: Luger, Berlin		
14:00 – 14:20	Poster 1	Erker, Münster / Grimme, Münster (lecture by Ugolotti) <i>Experimental Electron Density in Unusually Structured Organometallic Compounds</i>
14:20 – 14:40	Poster 2	Strohmann, Dortmund <i>The experimental charge density distribution as a key to the understanding of structure/reactivity patterns of alkyllithium and benzyllithium compounds</i>
14:40 – 15:00	Poster 3	Stalke, Göttingen <i>Electron density distribution in lithium organics</i>
15:00 – 15:20	Poster 4	Lentz, Berlin / Paulus, Berlin <i>Charge Density and Topological Properties of Boranes and their Lewis Acid Base Adducts</i>
15:20 – 15:40	Poster 5	Braunschweig, Würzburg <i>Electron density distribution in borylene complexes</i>
15:40 – 16:10		Coffee Break
Chair: Scherer, Augsburg		
16:10 – 16:30	Poster 6	Kaupp, Würzburg <i>Analysis of charge distributions in polar metal-ligand bonds</i>
16:30 – 16:50	Poster 7	Kohout, Dresden / Wagner, Dresden <i>Metal-metal and metal-ligand interactions from a viewpoint of direct space functionals</i>
16:50 – 17:10	Poster 8	Mitzel, Bielefeld <i>Electron density topology and nature of bonding in small ring compounds with dative bonds</i>

17:10 – 17:30	Poster 9	Krossing, Freiburg <i>Experimental charge densities of weakly bound complexes: Dispersive interactions and influence of relativity on calculated charge densities</i>
17:30 – 17:50	Poster 10, 11, 12	Englert, Aachen / Lehmann, Mühlheim <i>Experimental electron density studies of secondary interactions in solids</i>
17:50 – 19:30		Dinner
19:30 – 21:00		Poster Session

Thursday, February 05th, 2009

08:00 – 09:00		Breakfast
Chair: Luger, Berlin		
09:00 – 09:20	Poster 13	Koritsanszky, Murfreesboro <i>Methodological Developments in X-ray Charge Density Determination</i>
09:20 – 09:40	Poster 14	Dittrich, Göttingen <i>Using molecular dynamics for understanding and modelling disordered crystal structures</i>
09:40 – 10:00	Poster 15	Engels, Würzburg <i>Using quantum chemical computations to study the electron density and its influence on the reactivity</i>
10:00 - 10:20		Coffee Break
10:20 – 10:40	Poster 16	van Smaalen, Bayreuth <i>The maximum entropy method for accurate charge-density studies, and its application to proteins and other molecules of biological interest</i>
10:40 – 11:00	Poster 17	Schirmeister, Würzburg <i>Correlation of electron density derived molecular properties with biological activity - a new tool in rational ligand design</i>
11:00 – 12:30		Poster Session
12:30 – 14:00		Lunch
Chair: Stalke, Göttingen		
14:00 – 14:30	Poster 18, 19, 20	Eickerling, Augsburg / Himmel, Heidelberg / Scherer, Augsburg <i>On the Nature and Origin of Ligand-induced Charge Concentrations: The Key for Controlling C-H Activation Processes in Electron-Rich Transition Metal Complexes</i>
14:30 – 14:50	Poster 21	Fueß, Darmstadt <i>Correlated momentum, charge and magnetization density in the kagome staircase system $\text{Co}_3\text{V}_2\text{O}_8$</i>

14:50 – 15:10	Poster 22	Borrmann, Dresden / Pietsch, Siegen <i>Charge density response to an external high electric field</i>
15:10 – 15:30	Poster 23	Fueß, Darmstadt / Weyrich, Konstanz <i>The Electronic Structure of TiO₂, VO₂ and Related Transition-Metal Oxides: A Joined Electron-Density Study of Materials in Position, Momentum and Phase Space</i>
15:30 - 16:00		Coffee Break
Chair: Stalke, Göttingen		
16:00 – 16:20	Poster 24, 25	Pöttgen, Münster / Scherer, Augsburg (lecture by Hofmann) <i>Chemical bonding in rare earth–transition metal–carbides, borides, boride carbides, silicides, and pnictide oxides</i>
16:20 – 16:40	Poster 26	Grin, Dresden <i>Electron density and chemical bonding in intermetallic borides and structural analogues</i>
16:40 – 17:00	Poster 27	Rosner, Dresden <i>Electron densities of intermetallic compounds inspected by spectroscopy</i>
17:00 – 17:30	Poster 28	Jansen, Stuttgart / Paulus, Berlin / Weyrich, Konstanz <i>Deviations from Ideal Structures in Metallic Elements and Simple Intermetallics: Combined Experimental and Theoretical Studies of Electron distributions</i>
17:30 – 17:50	Poster 29	Fässler, Garching <i>Accurate charge density determination in Zintl phases</i>
17:50 –		Dinner and Beer

Departure for applicants (optional)

Friday, February 06th 2009

8:00 – 9:00	Breakfast
9:00	Referee Board Meeting

Departure

General remarks:

The allocated time slot to present each project is 20 minutes in general. Those projects combining various groups and methods got 10 minutes extension to present their common proposal. The slot accommodates a 15 (20) minutes presentation plus 5 (10) minutes of discussion.

It is the group's responsibility to identify the person to present the project, however, at the end all applicants should enter the stage to answer the referee's questions.

The sessions will be chaired to avoid delays according to the program.

The presentations ought to be given using overhead transparencies, slides, or PowerPoint presentations.