Preliminary Program SPP 1807 Workshop

Monday, October 19th, 2015

09:30 – 10:10	**Welcome Coffee**
10:10 – 10:20	**Opening**
	Chair: Martin Suhm
10:20 – 10:45	**L. Ackermann:** Control of London Dispersion Interactions in Metal Catalyzed C-H Activation
10:45 – 11:10	**A. Berkessel:** Dispersion Interaction in Metal- and Organocatalysis - Assessment and Implementation in Salalen Ligands and N-Heterocyclic Carbenes
11:10 – 11:35	**G. Clever / R. Mata:** Experimental and Computational Insights into Dispersion Interactions in Self-Assembled Supramolecular Host-Guest Systems
11:35 – 12:00	**H. Zipse (Vertr. P. Patschinski):** Dispersion-Directed Lewis Base Catalysis
12:00 – 13:00	Lunch
	Chair: Ricardo Mata
13:00 – 13:25	**M. Schnell:** Investigating dispersion interactions using broadband rotational spectroscopy - towards supramolecular design principles
13:25 – 13:50	**B. Friedrich / A. Slenczka:** Configurations of van der Waals complexes controlled via London dispersion forces as revealed by means of Stark spectroscopy in He-nanodroplets
13:50 – 14:15	**M. Gerhards:** Dispersion interactions in isolated molecules and molecular aggregates analyzed by IR/UV and Raman/UV double resonance spectroscopy
14:15 – 14.40	**R. Ludwig / S. Verevkin:** Quantifying dispersion forces in protic ionic liquids and their mixtures by means of low frequency spectroscopy and thermodynamic methods
14:40 – 15:05	**M. Suhm:** London vs. Keesom and Debye forces: From FTIR cluster spectroscopy of organic alcohols and ethers towards design principles of molecular recognition
15:05 – 15:30	**Coffee Break**

Chair: Stefan Grimme

15:30 – 15:55 **Invited Talk**
David Sherrill:
Quantifying interactions between functional groups using fragment symmetry adapted perturbation theory

15:55 – 16:40 **H. Bettinger:**
Dispersion driven isomerism in sigma-bonded acene dimers

16:40 – 17:05 **A. A. Auer /M. Mehring:**
Heavy main group elements as dispersion energy donors - experimental and theoretical studies of bismuth compounds with bismuth-pi-interactions as structure determining component

17:05 – 17:30 **R. J. F. Berger / N. W. Mitzel:**
Intramolecular dispersive interactions in the gas phase: experimental reference data and comparison with solid state and theory

17:30 – 18:00 **Break**

18:00 – 20:00 **Poster session**

Tuesday, October 20th, 2015

Chair: Lutz Ackermann

09:05 – 09.30 **W. Nau:**
London Dispersion Interactions inside Macrocycles

09.30 – 9:55 **P. Chen:**
Large Dispersion Effects in Organic and Organometallic Thermochemistry, Stereochemistry, and Reaction Mechanisms

9:55 – 10.20 **A. Görling / S. Tsogoeva:**
Dispersion Effects on Reactivity and Chemo-, Regio- and Stereoselectivity in Organocatalysed Domino Reactions: A Joint Experimental and Theoretical Study

10.20 – 10.45 **Coffee Break**

Chair: Lutz Ackermann

10:45 – 11:10 **P. R. Schreiner:**
London Dispersion as a design element to control molecular structures and chemical reactivity

11:10 – 11:35 **M. Tamm:**
Stabilization through dispersion interactions? Synthesis and characterization of coordinatively unsaturated metal complexes containing weakly coordinating anionic N-heterocyclic carbene ligands (WCA-NHC) showing metal N-arene interactions

11.35 – 12.00 **W. M. Klopper / S. Leutwyler:**
Combined experimental and theoretical determination of accurate bond energies of dispersion-dominated systems in the gas phase

12:00 – 13:00 **Lunch**

Chair: Peter Schreiner

13:00 – 13:25 **S. Grimme:**
Modeling of London Dispersion Interactions in Molecular Chemistry

13:25 – 13:50 **A. Heßelmann:**
Range-separated intermolecular perturbation theory with embedding for studying intramolecular interactions

13:50 – 14:15 **G. Jansen / S. Schulz:**
Range-separated intermolecular perturbation theory with embedding for studying intramolecular interactions

14:15 – 14:40 **Coffee Break**

Chair: Peter Schreiner

14:40 – 15:05 **F. Neese:**
Insight into weak intermolecular interactions from small to large systems using accurate wavefunction based ab initio and valence bond methods

15:05 – 15:30 **A. Tkatschenko:**
Understanding the Role of Dispersion Interactions in the Mechanical Properties of Molecular Crystals

15:30 - 16:00 **Discussion and concluding remarks**