Program Workshop Research Area A - 02.12.2014 Saal 1

RESOLV
RUHR EXPLORES SOLVATION
CLUSTER OF EXCELLENCE - EXC 1069

08:30 - 09:00	Put up posters	
09:00 - 09:10	**Welcome and overview Research Area A - Wolfram Sander**	
Chair: Sander		
09:10 - 09:30	**Lukasz Walewski** *"Computing the Local Superfluidity in Solvation Shells of Molecules in Helium"*	
09:30 - 09:50	**Matin Kaufmann** *"Observation of glycine in helium nanodroplets: From the neutral towards the zwitterion"*	
09:50 - 10:10	**Daniel Leicht** *"IR spectroscopy of solvated radicals in helium nanodroplets"*	
10:10 - 10:30	**Eike Spielberg** *"New ionic liquids for the preparation of coated ionogels"*	
10:30 - 11:00	Coffee break	
Chair: Merten		
11:00 - 11:50	**Hermann Weingärtner** *"Concepts of Ion Pairing"*	
11:50 - 12:10	**Anton Savitsky** *"Condensed Xenon as ideal solvent for highly-reactive species: An EPR study"*	
12:10 - 12:30	**Pandian Sokkar** *"Solvent effects on the relative stability of singlet and triplet diphenyl carbene: A QM/MM study"*	
12:30 - 15:00	Lunch & Poster Session	
Chair: Nürnberger		
15:00 - 15:20	**Nils Schulz** **"***Development of Ion-Pair-Based Chiral Halogen-Bond Donors for Asymmetric Catalysis"*	
15:20 - 15:40	**Christian Merten** *"Intermolecular interactions between chiral molecules in solution"*	
15:40 - 16:00	**Paolo Costa** *"The Highly Reactive Benzhydryl Cation Isolated and Stabilized in Water Ice"*	
16:00 - 16:30	Coffee break	
Chair: Weingärtner		
16:30 - 16:50	**Enrique Mendez Vega & Joel Mieres Perez** *"Understanding structure, reactivity and solvation of nitrenes"*	
16:50 - 17:10	**Patrick Nürnberger** *"Unraveling photochemical reaction pathways of diphenylcarbene in solvent mixtures"*	
17:10 - 17:30	**Ricardo Perez** *"Quantum (De)Localization in HCl/Water Cluetsrs at Ulrtralow Temperatures"*	
17:30 - 17:50	**Marie Holz** *"TranSOLV - from Basic to Applied Research"*	

POSTER - Workshop Research Area A
02.12.2014 - Veranstaltungszentrum (Saal1)

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1 *Solvent Influence on Cellulose Hydrolysis*
Claudia Loerbroks

2 *Paramagnetic Spin Systems in Condensed Xenon: EPR Characterization of Solvent Properties*
Thomas Lohmiller, Muralidharan Shanmugam, Paolo Costa, Wolfgang Lubitz, Wolfram Sander and Anton Savitsky

3 *Calculation of accurate single-electron redox potentials of organic molecules in aqueous solution*
Miho Isegawa

4 *Multidentate and Neutral Halogen-Bond-Donors: Applications in Supramolecular Chemistry and Catalysis*
David Bulfield

5 *Analysis of solvation in ionic liquids under high-pressure forced flow atmospheres with a modified measuring system*
Gerrit Dresp

6 *Carbene-Water Interactions: A QM/MM Study*
Miguel Fernandez-Oliva

7 *Solvent effects on the spin state of carbenes - a perspective*
Stefan Henkel

8 *Matrix isolation and solvation studies of diphenylmethyl radical*
Soumya Radhakrishnan

9 *Solvent effects on the spin state of carbenes - a perspective*
Linda Klute

10 *The Interaction of the Phenylchlorocarbene with Water. A Matrix Isolation Study*
Geneviève Richter

11 *Matrix Isolation and Spectroscopic Characterization of Naphthylnitrene-2-yl: a Quartet-ground- state Nitreno radical isolated in solid Argon*
Yetsedaw Tsegaw

12 *The Highly Reactive Benzhydryl Cation Isolated and Stabilized in Water Ice*
Paolo Costa

13 *Understanding structure and reactivity of high-spin nitrenes*
Enrique Mendez Vega

14 *Radicals and High-spin systems stabilized in conventional and non-conventional solvents at cryogenic temperatures.*
Joel Mieres Perez

15 *Isolation of the 9-fluorenyl cation*
Iris Trosien

16 *Imidazolium Ionic Liquids: A study on N-Hetero Cyclic Carbenes*
Bishnu Prasad Kar

17 *Concept of Mechanoswitching in Bergman Cyclization and Matrix Isolation Spectroscopy*
Kadam Pritam

18 Quantum *Simulations of Molecular Aggregates in Superfluid Helium*
Lukasz Walewski, Harald Forbert and Dominik Marx