Program Workshop Research Area B - 11.11.2014



08:30 -	09:00	Put up posters
09:00 -	09:10	Welcome and overview Research Area B - Roland Winter
Chair: Simon Ebbinghaus		
09:10 -	09:30	Michael Senske "Protein Stabilization by Macromolecular Crowding through Enthalpy rather than Entropy"
09:30 -	09:50	Mattias Heyden "Crowded Environments: Monte Carlo Simulations of 100-1000 Flexible Biopolymers in Solution"
09:50 -	10:10	Mirko Erlkamp "Intermolecular Interactions in Highly Concentrated Protein Solutions upon Compression and the Role of the Solvent"
10:10 -	10:30	Yao Xu "Water Dynamics in AOT Reverse Micelles "
10:30 -	11:00	Coffee break
Chair: Roland Winter		
11:00 -	11:20	Sho Imoto "TMAO Solutions at Ambient Conditions and Beyond"
11:20 -	11:40	Salome Pataraia "Influence of Temperature, Pressure, Co-solvents and Crowding on the Structure and Stability of a Small RNA Hairpin"
11:40 -	12:00	Christopher Rosin "Cosolvent and Crowding Effects on the Polymerization Kinetics of Actin"
12:00 -	12:20	Anna Kupka "Influence on the Crystallisation Process of Amino Acids from Solutions"
12:20 -	12:40	Elena Decaneto "Influence of Co-solvents, Light Control and Metal Substitution on the Enzymatic Activity of a Metalloproteinase"
12:40 -	13:45	Lunch
Chair: Matthias Heyden		
13:45 -		Marie Holz "TranSOLV - from Basic to Applied Research"
13:45 -		Marie Holz
13:45 -	14:05	Marie Holz "TranSOLV - from Basic to Applied Research" Alexander Esser
13:45 - 14:05 -	14:05 14:25	Marie Holz "TranSOLV - from Basic to Applied Research" Alexander Esser "From Glycine to Valine: Understanding THz Spectra of Biomolecular Building Blocks" Hendrik Vondracek
13:45 - 14:05 - 14:25 -	14:05 14:25 14:45	Marie Holz "TranSOLV - from Basic to Applied Research" Alexander Esser "From Glycine to Valine: Understanding THz Spectra of Biomolecular Building Blocks" Hendrik Vondracek "THz Spectroscopy for the Study of Solvation under Extreme Conditions" Felipe Conzuelo "Redox-Hydrogel Embedded Hydrogenase and Photosystem 1: Study of Properties and
13:45 - 14:05 - 14:25 - 14:45 -	14:05 14:25 14:45 15:05 15:25	Marie Holz "TranSOLV - from Basic to Applied Research" Alexander Esser "From Glycine to Valine: Understanding THz Spectra of Biomolecular Building Blocks" Hendrik Vondracek "THz Spectroscopy for the Study of Solvation under Extreme Conditions" Felipe Conzuelo "Redox-Hydrogel Embedded Hydrogenase and Photosystem 1: Study of Properties and Applications" Nicolas Plumeré "Electrochemical Investigations of Solvent Effect on Photosynthetic Proteins - Hydrogels vs. Protein
13:45 - 14:05 - 14:25 - 14:45 - 15:05 - 15:25 -	14:05 14:25 14:45 15:05 15:25	Marie Holz "TranSOLV - from Basic to Applied Research" Alexander Esser "From Glycine to Valine: Understanding THz Spectra of Biomolecular Building Blocks" Hendrik Vondracek "THz Spectroscopy for the Study of Solvation under Extreme Conditions" Felipe Conzuelo "Redox-Hydrogel Embedded Hydrogenase and Photosystem 1: Study of Properties and Applications" Nicolas Plumeré "Electrochemical Investigations of Solvent Effect on Photosynthetic Proteins - Hydrogels vs. Protein Monolayers"
13:45 - 14:05 - 14:25 - 14:45 - 15:05 - 15:25 -	14:05 14:25 14:45 15:05 15:25	Marie Holz "TranSOLV - from Basic to Applied Research" Alexander Esser "From Glycine to Valine: Understanding THz Spectra of Biomolecular Building Blocks" Hendrik Vondracek "THz Spectroscopy for the Study of Solvation under Extreme Conditions" Felipe Conzuelo "Redox-Hydrogel Embedded Hydrogenase and Photosystem 1: Study of Properties and Applications" Nicolas Plumeré "Electrochemical Investigations of Solvent Effect on Photosynthetic Proteins - Hydrogels vs. Protein Monolayers" Coffee break
13:45 - 14:05 - 14:25 - 14:45 - 15:05 - 15:25 - Chair: Ch	14:05 14:25 14:45 15:05 15:25 15:55 ristian F	Marie Holz "TranSOLV - from Basic to Applied Research" Alexander Esser "From Glycine to Valine: Understanding THz Spectra of Biomolecular Building Blocks" Hendrik Vondracek "THz Spectroscopy for the Study of Solvation under Extreme Conditions" Felipe Conzuelo "Redox-Hydrogel Embedded Hydrogenase and Photosystem 1: Study of Properties and Applications" Nicolas Plumeré "Electrochemical Investigations of Solvent Effect on Photosynthetic Proteins - Hydrogels vs. Protein Monolayers" Coffee break Hermann Victor Munoz
13:45 - 14:05 - 14:25 - 14:45 - 15:05 - 15:25 - Chair: Ch 15:55 -	14:05 14:25 14:45 15:05 15:25 ristian F 16:15	Marie Holz "TranSOLV - from Basic to Applied Research" Alexander Esser "From Glycine to Valine: Understanding THz Spectra of Biomolecular Building Blocks" Hendrik Vondracek "THz Spectroscopy for the Study of Solvation under Extreme Conditions" Felipe Conzuelo "Redox-Hydrogel Embedded Hydrogenase and Photosystem 1: Study of Properties and Applications" Nicolas Plumeré "Electrochemical Investigations of Solvent Effect on Photosynthetic Proteins - Hydrogels vs. Protein Monolayers" Coffee break Hermann Victor Munoz "Computational Insights on the Impact of Organic Cosolvents in Enzyme Stability" Fabian Klumpers
13:45 - 14:05 - 14:25 - 14:45 - 15:05 - 15:25 - 15:55 - 16:15 -	14:05 14:25 14:45 15:05 15:25 15:55 ristian F 16:15 16:35	Marie Holz "TranSOLV - from Basic to Applied Research" Alexander Esser "From Glycine to Valine: Understanding THz Spectra of Biomolecular Building Blocks" Hendrik Vondracek "THz Spectroscopy for the Study of Solvation under Extreme Conditions" Felipe Conzuelo "Redox-Hydrogel Embedded Hydrogenase and Photosystem 1: Study of Properties and Applications" Nicolas Plumeré "Electrochemical Investigations of Solvent Effect on Photosynthetic Proteins - Hydrogels vs. Protein Monolayers" Coffee break Herrmann Victor Munoz "Computational Insights on the Impact of Organic Cosolvents in Enzyme Stability" Fabian Klumpers "Solvent's Impact on Enzymatic Reactions" Lars Schäfer "Molecular Thermodynamics of Trypsin - Inhibitor Binding from Computational Alchemy"
13:45 - 14:05 - 14:25 - 14:45 - 15:05 - 15:55 - 16:15 - 16:35 -	14:05 14:25 14:45 15:05 15:25 ristian F 16:15 16:35 16:55	Marie Holz "TranSOLV - from Basic to Applied Research" Alexander Esser "From Glycine to Valine: Understanding THz Spectra of Biomolecular Building Blocks" Hendrik Vondracek "THz Spectroscopy for the Study of Solvation under Extreme Conditions" Felipe Conzuelo "Redox-Hydrogel Embedded Hydrogenase and Photosystem 1: Study of Properties and Applications" Nicolas Plumeré "Electrochemical Investigations of Solvent Effect on Photosynthetic Proteins - Hydrogels vs. Protein Monolayers" Coffee break Victor Munoz "Computational Insights on the Impact of Organic Cosolvents in Enzyme Stability" Fabian Klumpers "Solvent's Impact on Enzymatic Reactions" Lars Schäfer "Molecular Thermodynamics of Trypsin - Inhibitor Binding from Computational Alchemy" Pandian Sokkar "Hybrid Quantum Mechanics/Molecular Mechanics/Coarse Grained Modeling: A Triple-Resolution
13:45 - 14:05 - 14:25 - 14:45 - 15:05 - 15:25 - 16:15 - 16:35 - 16:55 -	14:05 14:25 14:45 15:05 15:25 ristian F 16:15 16:35 16:55 17:15 17:15	Marie Holz "TranSOLV - from Basic to Applied Research" Alexander Esser "From Glycine to Valine: Understanding THz Spectra of Biomolecular Building Blocks" Hendrik Vondracek "THz Spectroscopy for the Study of Solvation under Extreme Conditions" Felipe Conzuelo "Redox-Hydrogel Embedded Hydrogenase and Photosystem 1: Study of Properties and Applications" Nicolas Plumeré "Electrochemical Investigations of Solvent Effect on Photosynthetic Proteins - Hydrogels vs. Protein Monolayers" Coffee break Vettor Munoz "Computational Insights on the Impact of Organic Cosolvents in Enzyme Stability" Fabian Klumpers "Solvent's Impact on Enzymatic Reactions" Lars Schäfer "Molecular Thermodynamics of Trypsin - Inhibitor Binding from Computational Alchemy" Pandian Sokkar "Hybrid Quantum Mechanics/Molecular Mechanics/Coarse Grained Modeling: A Triple-Resolution Approach for Biomolecular Systems" Frank Schulz

POSTER - Workshop Research Area B 11.11.2014 - Veranstaltungszentrum/Saal1



1 Sumit Mittal

"Influence of Molecular Environment on Biological Interactions"

- 2 Alexander Esser, Jian Sun, Harald Forbert, Dominik Marx "From Glycine to Valine: Understanding THz Spectra of Biomolecular Building Blocks"
- **3** Sho Imoto, Harald Forbert, Dominik Marx "TMAO Solutions at Ambient Conditions and Beyond"
- 4 Anna Kupka "Influence on the Crystallisation Process of Amino Acids from Solutions"
- 5 Michael Dirkmann "Exploring Solvent-Enzyme Interactions"
- 6 Fabian Klumpers "Protein Solvation at High Concentrations"
- 7 Nadja Berger "Conformational Studies on Cyclic Model Peptides"
- 8 Tatiana Vasilevskaya "Matrix Metalloproteienase-2: Modellung the Mechanism of Proteolysis"

9 Gopal Srinivasa

"Molecular Thermodynamics of Trypsin-Inhibitor Binding from Computational Alchemy"