

## Program Summer School Solvation Science 2024

**Tuesday, May 21<sup>st</sup> – @ ZEMOS 0.17/0.19**

09:00 – 09:30      *Registration*

09:30 – 09:35      *Welcome: Dr. Mario Wiesenfeldt*  
ECR Board & Ruhr-Universität Bochum

### *Solvation in Catalysis*

*Chair: Taritra Mukherjee*

09:35 – 10:35      **Dr. Maksim Plekhanov,**  
RWTH Aachen, DE  
*“Uncovering the local structure of liquids and disordered phases with pair distribution function analysis”*

10:35 – 11:00      **Coffee Break**

### *Solvation in Medicinal/Biomolecular Chemistry*

*Chair: Dila Kurtul*

11:00 – 12:00      **Prof. Dr. Amish Patel**  
University of Pennsylvania, USA  
*“Characterizing Protein Interactions to Inform its Interactions”*

12:00 – 13:30      **Lunch Break**

### *Afternoon: Welcome event: Excursion to Altena Castle*

13:30                      Bus transfer to the medieval hilltop castle of Altena

15:00                      Altena castle is one of the loveliest hilltop castles in Germany. For centuries it has sat enthroned up on the Wulfsegge and has been the eponym and symbol of Altena. Guided tour of the permanent exhibition, including an introduction to the history

of the Altena castle, a view at the castle chapel, as well as an insight into the lifestyle of knights and noblemen.

17:30 Welcome dinner “Road Stop Dortmund”

19:00 – 20:00 Return to RUB

## **Wednesday, May 22<sup>nd</sup> – @ ZEMOS 0.17/0.19**

09:00 – 09:05 *Welcome: Dr. Ana Vila Verde*  
ECR Board, University of Duisburg-Essen

### *Solvation in Catalysis*

*Chair: Taritra Mukherjee*

09:05 – 10:05 **Prof. Dr. Cristina Trujillo Del Valle**,  
The University of Manchester, UK  
*“Computational Insights into the Role of Solvent in Catalysis: Methods and Applications”*

### *Solvation in Green/Sustainable Chemistry*

*Chair: Sunita Mondal*

10:05 – 11:05 **Assoc. Prof. Ian C. Bourg**,  
Princeton University, US  
*“Why mud is sticky “*

11:05 – 11:30 **Coffee Break**

11:30 – 12:30 **Prof. Dr. Kristina Tschulik**  
Ruhr Universität Bochum, GER  
*“Advanced Electrochemical Methods to Guide the Design of Electrocatalysts “*

12:30 – 14:00 **Lunch Break**

14:00 – 15:00 **Prof. Dr. Elsa Sanchez Garcia**  
Technische Universität Dortmund, GER  
*“Computational Approach to Solvation in Drug Design”*

15:00 – 15:30 **Coffee Break**

## Solvation in Medicinal/Biomolecular Chemistry

**Chair: Dila Kurtul**

15:30 – 16:30      **Prof. Dr. Nick Le Brun**,  
University of East Anglia, UK  
*“Native mass spectrometry of metallo-proteins: mechanistic insights from desolvated gas phase ions”*

## Diversity event

**Chair: Dilber Tan**

16:30 – 17:00      **Ashwini (Ash) Walde**  
*“Inclusive Futures: Advancing Gender Equality in the Workplace”*

17:00 – 17:20      **Zhenya Landiak** *“Burnout culture: Reaction, Dealing, Prevention”*

17:20 – 17:30      Award Ceremony "Student Challenge Solvation Science", Dr. Mario Wiesenfeldt

17:30 – 18:30      **Poster session (international students)  
and parallel Get-together at the ZEMOS Foyer**

18:30 – 20:00      **Scientific movie night ID 04/445 (optional for participants)**  
*“iHUMAN: First we create technology, then it recreates us.”*  
  
An explosive real-life political thriller, iHUMAN gives deep access to the booming Artificial Intelligence (AI) industry. It illuminates how the most powerful and far-reaching technology of our time is changing our lives, our society and our future. iHUMAN asks us all: in an AI age, what does it mean to be human? From information control to deepfakes, iHUMAN gives unprecedented access to the experts on the frontlines of this technology, and unique insight into the minds that are leading the revolution. AI can make our lives easier, but at what cost?

## **Thursday, May 23<sup>rd</sup> – @ ZEMOS 0.17/0.19**

09:30 – 09:35      **Welcome: Dr. Martin Rabe**  
ECR Board, Max-Planck-Institut für Eisenforschung

## Solvation in Catalysis

**Chair: Taritra Mukherjee**

09:35 – 10:35      **Prof. Dr. Stefan Huber**  
Ruhr Universität Bochum, GER  
*“Halogen and Chalcogen Bonding in Solution”*

10:35 – 11:00 Coffee Break

### *Solvation in Medicinal/Biomolecular Chemistry*

*Chair: Dila Kurtul*

11:00 – 12:00 **PD Dr.-Ing. Christoph Held**  
Technische Universität Dortmund, GER  
*“Thermodynamics of Pharmaceutical Formulations”*

12:00 – 13:30 Lunch Break

### *Career Part*

*Moderator: Dr. Ana Vila Verde*

13:30 – 13:35 Welcome

13:35 – 14:05 **Annabelle Beyer, Stefan Weber, and Martin Bellof** – Chemstars & Start4Chem, Start-up and Entrepreneurship

14:05 – 14:35 **Dr. Desi Dobрева** – Entrepreneur at Mechanolution

14:35 – 15:05 **Dr. Sara Ghaisari** – Data Scientist at DISH Digital Solutions GmbH

15:05 – 15:35 Coffee Break

15:35 – 16:05 **Dr. Sneha M. Dixit** – Senior Scientist at AbbVie Deutschland GmbH & Co KG

16:05 – 16:35 **Dr. Mathies Evers** – Senior Product Development Engineer at thyssenkrupp nucera AG & Co. KGaA

16:35 – 18:00 Panel discussion with **Dr. Sara Ghaisari, Dr. Sneha M. Dixit, Dr. Mathies Evers, Dr. Desi Dobрева, and Chemstart&Start4Chem**

*Closing: Dr. Ana Vila Verde*

ECR Board, University of Duisburg-Essen

18:00 – 21:00 Get-together BBQ at Beckmanns Hof

**Friday, May 24<sup>th</sup>**

*RESOLV's participating institutes. [Advanced Laboratory Modules >](#)*