

# **Getting the Basics Right: Capacitance, Entropy and Stress of Electrified Solid/Liquid Interfaces**

**854. WE-Heraeus-Seminar**

**03 - 06 May 2026**

**at the Physikzentrum Bad Honnef, Germany**

**WILHELM UND ELSE  
HERAEUS-STIFTUNG**



# Program

**Sunday, 03 May 2026**

16:00 - 20:00 Registration

18:00 – 19:30 *BUFFET SUPPER and informal get-together*

19:30 – 20:00 Jun Huang,  
Aliaksandr  
Bandarenka,  
Kathleen Schwarz

**Welcoming Note & Video Presentation:  
“About the Wilhelm and Else Heraeus  
Foundation”**

20:00 - 20:45 Jörg Weißmüller

**Electrocapillary Coupling – Surface  
Phenomena and Implications for  
Materials Behavior**

# Program

**Monday, 04 May 2026**

07:30 - 08:45	<i>BREAKFAST</i>	
08:45 – 09:30	Galina Tsirlina	<b>Thermodynamics of the perfectly polarizable electrodes: complicating and less known issues</b>
09:30 - 10:00	Michael Eikerling	<b>Cracking the interface problem: going deep and wide with (almost classical) analytical theory</b>
10:00 – 10:30	Marcel Risch	<b>Measurement of Enthalpy and Entropy of the Cobaltite-Water Interface</b>
10:30 – 10:35	Conference Picture	
10:35 - 11:00	<i>COFFEE BREAK</i>	
11:00 - 11:30	Victor Climent	<b>Thermodynamic Characterization of Electrochemical Interphases on Noble Metal Single-Crystal Electrodes Using Temperature-Dependent and Laser-Induced Techniques</b>
11:30 - 11:50	Nicci Fröhlich	<b>The electric double layer structure of bare and ad-atom modified stepped platinum electrodes</b>
11:50 - 12:10	Jinwen Liu	<b>Multiscale Modeling of Surface Heterogeneity and Adsorbates effects on Electrochemical Interfaces</b>
12:10 – 12:30	Sudarshan Vijay	<b>Quantifying Electrical Double Layer Thermodynamics via 2D Periodic DFT and Machine Learning Interatomic Potentials</b>
12:30 – 14:00	<i>LUNCH</i>	

# Program

**Monday, 04 May 2026**

14:00 - 14:30	Jun Cheng	<b>AI acceleration of AIMD simulation of electrochemical interfaces</b>
14:30 - 15:00	Olaf Magnussen	<b>X-ray scattering studies of the molecular structure of the aqueous electrolyte near platinum electrodes</b>
15:00 – 15:30	Marko Melander	<b>Thermodynamics of water-metal interface formation from DFT-MD Simulations</b>
15:30 – 16:00	<i>COFFEE BREAK</i>	
16:00 – 16:30	Manuel Landstorfer	<b>Thermodynamic modelling of the electrode–electrolyte interface — Double-layer capacitance, solvation number, and validation</b>
16:30 – 17:00	Tao Wang	<b>EDL Structure at Potentials Significantly Deviated from the PZC</b>
17:00 – 18:30	POSTER FLASH	
18:30 – 20:00	<i>DINNER</i>	
From 20:00	POSTER SESSION	

# Program

**Tuesday, 05 May 2026**

07:30 - 08:45	<i>BREAKFAST</i>	
08:45 - 09:30	Tamas Pajkossy	<b>How to measure the double layer capacitance of electrocatalytic interfaces?</b>
09:30 – 10:00	Yitao Long	<b>Confinement controlled electrochemistry</b>
10:00 – 10:30	Jahan Dawlaty	<b>Dissecting the Electrochemical Response of the Double Layer into Spectroscopically Resolvable Molecular Dynamics</b>
10:30 - 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:30	Vanessa J. Bukas	<b>Entropy-enthalpy compensation in electrocatalytic rates</b>
11:30 – 11:50	Xinwei Zhu	<b>Understanding Cation effects in Alkaline Hydrogen Evolution Reaction: An Electrostatic Perspective</b>
11:50 – 12:10	Alfred Larsson	<b>Anomalous charging of platinum seen by X-ray spectroscopy</b>
12:10 – 12:30	Albert Engstfeld	<b>A Step Towards FAIR Electrochemical Data: A Database of Cyclic Voltammograms for Metal Single-Crystals</b>
12:30 – 14:00	<i>LUNCH</i>	

# Program

Tuesday, 05 May 2026

14:00 – 14:30	Guang Feng	<b>Interfacial Structure, Ion Transport, and Heat Generation in Electrified Solid/Liquid Interfaces</b>
14:30 – 15:00	Marco Schoenig	<b>Measuring the entropy of interface formation at Au(111)</b>
15:00 – 15:30	Nicolas G. Hörmann	<b>Charging, Chemisorption, and Water Structure at applied potential conditions: Insights from Atomistic Simulations</b>
15:30 – 16:00	<i>COFFEE BREAK</i>	
16:00 - 16:30	Chris-Kriton Skylaris	<b>Large-scale atomistic simulations of battery materials and interfaces</b>
16:30 – 17:00	Peter Dunne	<b>Magnetic Field Effects in the Electrochemical Double Layer</b>
17:00 – 18:00	<u>Moderator:</u> Aliaksandr Bandarenka	<b><u>PANEL DISCUSSION:</u></b> <b>Today's education and supervision in electrochemistry</b> <b>Panelists: Galina Tsirlina, Olaf Magnussen, Jörg Weißmüller, Jun Cheng</b>
18:30	<i>HERAEUS DINNER &amp; Poster Award Ceremony</i> <i>(social event with cold &amp; warm buffet with complimentary drinks)</i>	

# Program

**Wednesday, 06 May 2026**

07:30 - 08:45	<i>BREAKFAST</i>	
08:45 - 09:30	David Raciti	<b>Probing the Electrified Solid–Liquid Interface with Surface Stress, Spectroscopy, and Mass Spectrometry</b>
09:30 – 10:00	Jan Rossmeisl	<b>Electrocatalysis on alloys</b>
10:00 – 10:30	Matthew Gebbie	<b>Exploring how ionic correlations impact electric double layer formation and electrocatalytic activity</b>
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:30	Katharina Doblhoff-Dier	<b>Potential of zero (free) charge: Why we should care</b>
11:30 – 11:50	Xiao Yu Li	<b>The Breath of Solid-Liquid Interface during Electrocatalysis</b>
11:50 – 12:10	Alexander von Rueden	<b>Electrochemical free energy barriers from first principles</b>
12:10 – 12:30	Fabiola Dominguez Flores	<b>From Solvation to Capacitance: How Divalent-Ion Partial Charge Transfer Shapes the Compact Layer</b>
12:30 – 12:35	Scientific Organizers	<b>Closing Remarks</b>
12:35 - 14:00	<i>LUNCH</i>	

**End of the seminar and departure**