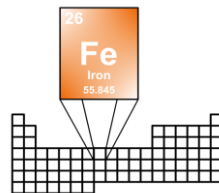




TECHNISCHE
UNIVERSITÄT
DARMSTADT



Understanding

Iron & friends!

CRC 1487 Symposium

03.-05.09.2024

Darmstadt, Germany

Tuesday, 03.09.2024

ARRIVAL (9:00 – 10:00)

10:00 – 12:10	CHAIR: Prof. Christian Hess	
10:00 – 10:15	Prof. Ulrike Kramm, Technische Universität Darmstadt	Welcome
10:15 – 11:00	Prof. Robert Schlögl, Alexander von Humboldt- Stiftung/Fritz-Haber-Institut der Max-Planck-Gesellschaft	Catalysis with Iron Surfaces: What is Special in Relation to Noble Metals
11:00 – 11:20	Hannah Lamers, Technische Universität Darmstadt	Iron-based catalysts for the selective Acetylene Hydrogenation
11:20 – 11:50	Dr. Bruno Chaudret, LPCNO INSA-CNRS Toulouse	Iron Based Nanoparticles for Magnetically Induced Catalysis

LUNCH

14:00 – 15:45	CHAIR: Prof. Vera Krewald	
14:00 – 14:45	Prof. Frank Neese, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr	Exploring High Valent Iron chemistry with a Combination of Quantum Chemistry and Spectroscopy
14:45 – 15:05	Carlos M. Jimenez-Muñoz, Technische Universität Darmstadt	Electronic structure of mononuclear iron phthalocyanine complexes in matrix isolation spectroscopy: experiment challenges theory
15:05 – 15:25	Mathias L. Skavenborg, University of Southern Denmark	Iron Complexes as Charge Carriers in All Iron Redox Flow Batteries
15:25 – 15:45	Dr. Young-Joon Song, Goethe-Universität Frankfurt Niklas von Rhein, Technische Universität Darmstadt	Computational Models for FeNC catalysts - A detailed view on electronic structures from molecular to periodic models

COFFEE BREAK

16:15 – 17:05	CHAIR: Prof. Christina Thiele	
16:15 – 16:45	Dr. ing. Daniël L. J. Broere, Utrecht University	A Tale of Two Irons: Synthesis and Reactivity of Well- defined Diiron Expanded Pincer Complexes
16:45 – 17:05	Dr. Stephan Müssig, Friedrich-Alexander-Universität Erlangen-Nürnberg	Control of magnetic dipole-dipole interactions in iron oxide-based supraparticles

GROUP PICTURE (17:05 – 17:15)

POSTER SESSION, Room 204 (17:15 – 19:15)

Wednesday, 04.09.2024

08:30 – 10.20		CHAIR: Prof. Jan Philipp Hofmann
08:30 – 09:00	Prof. Matthias Bauer, Universität Paderborn	Photoactive Iron complexes and time-resolved X-ray spectroscopy – New friends
09:00 – 09:20	Dr. Dimitrios Bessas, European Synchrotron Radiation Facility	Nuclear Resonance Scattering of synchrotron radiation for iron and its friends
09:20 – 09:40	Dr. Juliusz A. Wolny, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau	Insight into the Dynamics of Spin Crossover Transitions and Cooperativity with Nuclear Inelastic Scattering and Density Functional Theory
09:40 – 10:00	Sun Myung Kim, Technische Universität Darmstadt	Electronic Structure and Redox Properties of Iron in Different Environments Studied by Valence and Core Level Spectroscopies
10:00 – 10:20	Nicole Segura-Salas, Technische Universität Darmstadt	Manipulating FeNC model catalysts with metal nanoparticles: Effect on activity and selectivity for CO ₂ RR

COFFEE BREAK

10:50 – 12.20		CHAIR: Prof. Herbert Plenio
10:50 – 11:20	Prof. Christine McKenzie, University of Southern Denmark	Local Environment Influence on High Valent Non-heme Iron
11:20 – 11:40	Dr. Lukas Kaltschnee, Technische Universität Darmstadt	Transient intermediates of the [Fe]-hydrogenase catalysis characterized by sensitivity-enhanced NMR
11:40 – 12:00	Jun.-Prof. Alicia Casitas, Philipps-Universität Marburg	High-Valent Organometallic Iron Complexes
12:00 – 12:20	Justin Krampe, Technische Universität Darmstadt	Analysis of spin interactions in μ -oxo bridged copper, nickel and iron di-nuclear complexes

LUNCH

14:00 – 16.00		CHAIR: Prof. Angela Möller
14:00 – 14:30	Prof. Martin Muhler, Ruhr Universität Bochum	Selective Catalytic Oxidation of Alcohols and Olefins over Cobalt-based Spinel and Perovskite Nanoparticles
14:30 – 14:50	Prof. Oliver Clemens, Universität Stuttgart	Fe-containing perovskites – Topochemistry and a Playground of Functional Properties
14:50 – 15:10	Hannah Wilhelm, Technische Universität Darmstadt Jan Welzenbach, Technische Universität Darmstadt	Mechanistic insight into iron molybdate catalysts during oxidative dehydrogenation using coupled operando spectroscopy and diffraction
15:10 – 15:30	Dr. Michael Lammer, Graz University of Technology	Iron-based oxygen carrier development for hydrogen production and purification
15:30 – 16:00	Prof. Jan-Dierk Grunwaldt, Karlsruher Institut für Technologie	Looking at iron and friends at work: Fascinating elements for catalysis and X-rays

COFFEE BREAK (16:00 – 16:30)

CITY TOUR (16:30 –18:30)

CONFERENCE DINNER (from 20:00)

Thursday, 05.09.2024

08:30 – 10.35

CHAIR: Prof. Ulrike Kramm

08:30 – 09:15

Dr. Deborah J. Myers,
Argonne National Laboratory

Iron-based catalysts for proton-exchange membrane fuel cells and anion-exchange membrane water electrolyzers

09:15 – 09:35

Prof. Jörg Schneider,
Technische Universität Darmstadt

Isolating single iron-nitrogen centers in carbon nanostructures

09:35 – 09:55

Mohsin Muhyuddin,
University of Milano-Bicocca

Evolution of Active Sites in Iron Phthalocyanine Functionalized Carbon during Pyrolysis: Transforming into Active Fe-N_x-C Electrocatalysts for Oxygen Reduction Reaction

09:55 – 10:15

Julia Buschermöhle,
Deutsches Zentrum für Luft- und Raumfahrt e. V.

High-performance MOF-based Fe-Sn-N-C catalysts for the ORR in HT-PEM fuel cells

10:15 – 10:35

Dr. Kaltum Abdiaziz,
Max-Planck-Institut für Chemische
Energiekonversion, Mülheim an
der Ruhr
Dr. Lingmei Ni,
Technische Universität Darmstadt

Spectroelectrochemical EPR and Mössbauer for Identifying Active Sites in FeNC Catalysts.

COFFEE BREAK

11:05 – 12:45

CHAIR: Prof. Rolf Schäfer

11:05 – 11:35

Prof. Jasnamol Palakkal,
Georg-August-Universität
Göttingen

Growth Optimization of Fe-based Epitaxial Tellurides Using Hybrid PLD

11:35 – 11:55

Dr. Imants Dirba,
Technische Universität Darmstadt

Upgrading magnetism of iron by interstitial nitrogen

11:55 – 12.15

Giovanni d'Andrea,
Technische Universität Darmstadt

Materials Science of Nitrogen Ion Implantation in α -Fe

12.15 – 12.45

Concluding Remarks

LUNCH