



Newsletter

Spring 2023



Research Highlights

[Click here](#) to take a brief look at what researchers at UniSysCat have been working on the past few months.



Current Affairs

[Click here](#) to view the most recent events, awards and other affairs hosted by UniSysCat.



Upcoming Events

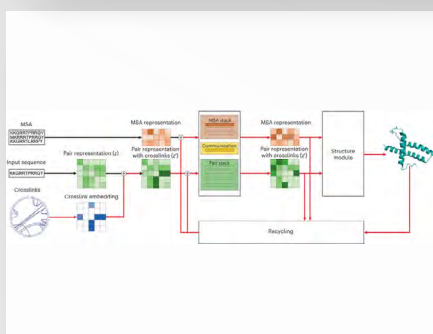
[Click here](#) to take a look at the colloquiums and other events coming up.

Research Highlights



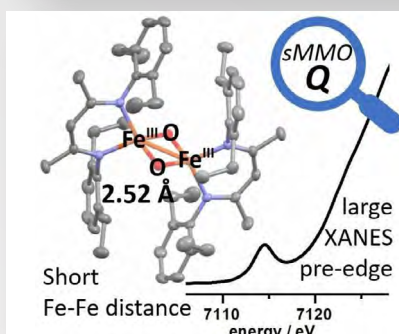
Doubling the Insights in the Dynamics of Nature's Oxygen Evolution

Two outstanding publications from scientists of the research networks UniSysCat and the CRC 1078 provide new atomistic insights on the dynamics and mechanism of Nature's way to produce the atmospheric oxygen, using complementary methodical approaches.



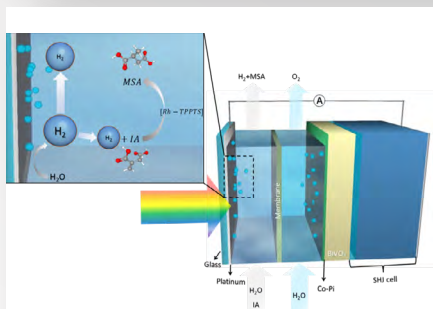
AlphaLink – made by double excellence

In a joint effort, the Rappsilber and the Brock group stemming from the two clusters of excellence UniSysCat and SClol developed a new prediction tool, AlphaLink, for challenging protein structure targets by combining experimental data and deep learning.



A Biologically Relevant $[\text{Fe}_2(\mu\text{-O})_2]$ Diamond Core Motif with a Short Iron-Iron Distance

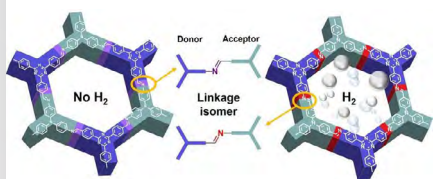
The groups of T. Braun, H. Dau, C. Limberg, M. Driess and K. Ray report the synthesis and characterization of an O_2 -derived four-coordinate $[\text{Fe}_2(\mu\text{-O})_2]^{2+}$ complex and show that lower coordination number for the irons allow for more flexibility in the diamond core than previously proposed.



A Photo Tandem Reaction – Hydrogen transfer from Water to chemical products

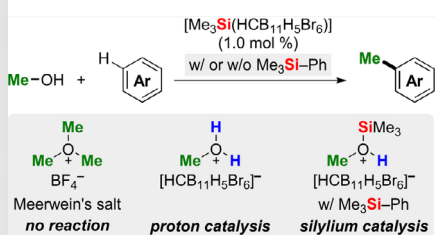
The groups of van de Krol and Schomäcker have evaluated the life cycle net energy assessment of sustainable H_2 production and hydrogenation of chemicals in a coupled photoelectrochemical device.

Research Highlights



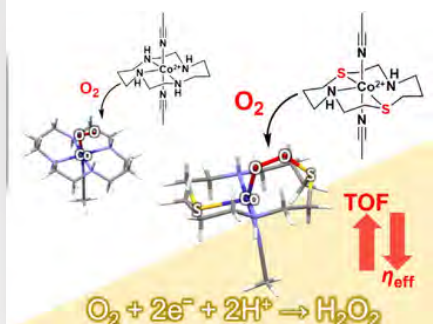
Small change – big effect ...

For a joint publication the five UniSysCat group of Shuang Li, Reinhard Schomäcker, Roel van de Krol, Peter Saalfrank and Arne Thomas teamed up to elucidate the impact of the orientation of a single functional group in a photocatalyst on its catalytic performance.



Catalytic Protocol for Direct Methylation of Arenes with Methanol

The Oestreich group has found a new catalytic protocol for Friedel-Crafts C(sp²)-H methylation with methanol through the use of catalytically generated Meerwein's salt-type oxonium ions.



Jointly achieved insights in different roles of thiolates in bioinorganic chemistry

The three Unisyscat Groups (Hildebrandt, Dau and Ray) reveal in two joint publications the vital role of sulfur as non-innocence ligand in the catalytic reduction of dioxygen to hydrogen peroxide and in mimicking the reactivity of class Ib ribonucleotide reductases (RNRs).

Current Affairs



Renske M. van der Veen appointed as W2-S professor at the TU Berlin

Prof. Renske M. van der Veen she has been officially appointed for a joint W2-S professorship with the Technische Universität Berlin at the Institute of Optics and Atomic Physics in the field of “Dynamics in Light Energy Conversion”. Congratulations!



Farewell to Fire?

A joint live event with the chemist and philosopher PD Dr. Jens Soentgen from Augsburg University and the artist Julius von Bismark from Berlin, which was organized by Dr. Benjamin Steininger from the cluster of excellence UniSysCat

Upcoming Events



FAIR Research Data Management: Basics for Chemists

Entry-level workshop for good Research Data Management (RDM).

Date: 22-23.05.23, TU Berlin

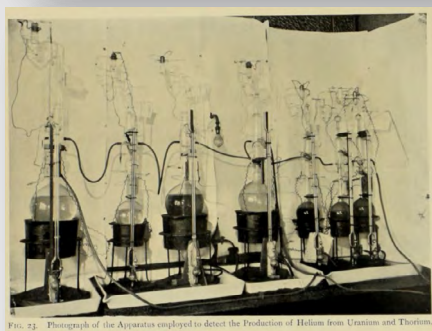


FIG. 23. Photograph of the Apparatus employed to detect the Production of Helium from Uranium and Thorium.

Special Colloquium

“Chemical Geography: a non-existent field?” will be presented as a lecture by Prof. Dr. Andrew Barry from the University College London.

Date: 22.05.23, 05:15 pm, TU Berlin



Special Colloquium jointly organized by UniSysCat and CRC1078

“A Possible Light-Independent Role for Microbial Rhodopsins in Building the Lipid Bilayer” will be presented by Prof. Katrina Forest.

Date: 25.05.2023, 05:15 pm



UniSysCat - Colloquium

“Theoretical description of the catalytic actions of CO-dehydrogenases and hydrogenases: tackling the challenges of reliable QM/MM modelling” will be presented by Prof. Claudio Greco.

Date: 14.06.2023, 05:15 pm, TU Berlin & online

Upcoming Events



Long Night of Sciences - Pub Quiz

Join us for a quiz evening in the TU tent, jointly organized by all seven Clusters of Excellency in Berlin. In the pub quiz, we ask questions from all areas of research in these Clusters. The event will be held in German.

Date: 17.06.2023, 08:30 pm, TU Berlin



Workshop: RDM School of Catalysis

The workshop will cover all relevant aspects of RDM in the applied workflows in catalysis as well as practical advice, guidelines and tools, such as electronic lab notebooks. As the workshop is beginner friendly, no prior knowledge of RDM is required.

Date: 31.07.23, TU Berlin



UniSysCat - Colloquium

Prof. Carsten Streb from the Johannes Gutenberg University, Mainz, will be holding a lecture on the topic “Molecular metal oxides for energy conversion and storage”.

Date: 09.08.23, 05:15 pm, TU Berlin & online



Imprint

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