

Univerza
v Ljubljani

Fakulteta *za kemijo*
in kemijsko tehnologijo

p.p. 537, Večna pot 113
1001 Ljubljana
telefon: 01 479 80 00
faks: 01 241 91 44
dekanat@fkkt.uni-lj.si



VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI / INVITATION TO THE
LECTURE WITHIN DOCTORAL PROGRAMME IN
CHEMICAL SCIENCES

Prof. Dr. Stefan Bräse

Karlsruhe Institute of Technology (KIT), Karlsruhe

z naslovom / title:

**A trip into the blue - OLED research as an
example of digitalization in chemistry**

v sredo, 14. 2. 2024 ob 15. uri /

on Wednesday, 14. 2. 2024 at 15.00

**v predavalnici 1 v 1. nadstropju Fakultete za kemijo in
kemijsko tehnologijo, Večna pot 113 / in lecture room 1,
1st floor at the Faculty of Chemistry and Chemical
Technology, Večna pot 113**

Vljudno vabljeni! | Kindly invited!

Abstract:

This talk will describe our vision of digital and automated chemistry to facilitate and accelerate scientific work. As an experimental chemistry group, our work processes include designing, synthesizing, and analyzing small to medium-sized organic (sometimes metal-organic) molecules. Limited by the traditional work environments in the form of lab processes, hardware, and software, we decided to develop mechanisms to improve our work's efficiency, reproducibility, and openness. The components of our current strategy include the development and integration of software to enable research data management (RDM) workflows for FAIR (findable, accessible, interoperable, and reusable) data and the implementation of automation concepts to standardize and improve all experimental aspects of our work. The different elements of a digital research data management strategy are described, particularly the electronic lab notebook Chemotion ELN, the repository Chemotion, and other software components. With a few selected examples, we highlight the conversion of data to standardized file formats, the extraction of metadata, and the analysis of chemical analytical data with embedded, open-source components. [1-4] The combination of digitalization strategies with automated processes is depicted with examples of the platform ChemASAP. ChemASAP, currently under construction as a research infrastructure at KIT, will allow the automated synthesis of chemical entities - combining high throughput synthesis, reproducible scientific experiments, and -in the long run- establishing large databases dedicated to support scientists with sophisticated data analysis tools. [5]

The second part deals with our OLED research research, featuring TADF effects and synthetic paracyclophane chemistry. [6]

Literature:

[1] F. Tristram, N. Jung, P. Hodapp, R. Schröder, C. Wöll, S. Bräse, *Adv. Funct. Mat.* 2024, in press. The Impact of Digitalized Data Management on Material System Workflows - 10.1002/adfm.202303615. [2] P. Tremouilhac, A. T. C. Nguyen, Y.-C. Huang, S. Kotov, D. Lütjohann, F. Hübsch, N. Jung, S. Bräse, *J. Cheminform.* 2017, 9, 54. Chemotion ELN: An Open Source Electronic Lab Notebook for chemists in academia - 10.1186/s13321-017-0240-0. [3] P. Tremouilhac, C.-L. Lin, P.-C. Huang, Y.-C. Huang, A. Nguyen, N. Jung, F. Bach, R. Ulrich, B. Neumair, A. Streit, S. Bräse, *Angew. Chem.* 2020, 22771-22778. The repository Chemotion: infrastructure for sustainable research in chemistry - 10.1002/anie.202007702. [4] P. Tremouilhac, P.-C. Huang, C.-L. Lin, Y.-C. Huang, A. Nguyen, N. Jung, F. Bach, S. Bräse, *Chem. Meth.* 2021, 8-11. Chemotion repository, a curated repository for reaction information and analytical data - 10.1002/cmtd.202000034. [5] <https://www.knmf.kit.edu/#Anker2>; <https://fms.ibcs.kit.edu> [6] G. Hong, X. Gan, C. Leonhardt, Z. Zhang, J. Seibert, J. Busch, S. Bräse, *Adv. Mat.* 2021., e2005630. A brief History of OLEDs - Emitter Development and Industry Milestones DOI:10.1002/adma.202005630