



Martedì 28 Ottobre 2025, ore 14:30.

in

Aula Seminari del Dipartimento di Scienze e Tecnologie
Chimiche

Il Prof. Stefan Bräse

Institute of Biological and Chemical Systems- Functional Molecular Systems (IBCS-FMS), and Institute of Organic Chemistry (IOC), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

e

la Prof.ssa Ute Schepers

*Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT),
Karlsruhe, Germany*

terranno un doppio seminario intervallato da pausa caffè
sulla

Transizione digitale

In particolare:

“Digital Chemistry- a trip to the blue”

e

**“Self-driving labs for the accelerated
discovery of novel materials for health
technologies”**



Digital chemistry – A trip to the blue

Prof. Dr. Stefan Bräse

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Self-driving labs for the accelerated discovery of novel materials for health technologies

Prof. Dr. Ute Schepers

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Karlsruhe Institute of Technology, Karlsruhe

The digital transformation of chemistry is redefining how molecules are designed, synthesized, and understood. Advances in data-driven tools, automation, and artificial intelligence are enabling a new research paradigm — one where chemical discovery is faster, more reproducible, and more accessible than ever before. This joint lecture will present two complementary perspectives on how digital technologies and autonomous systems are reshaping molecular science and its applications in health technologies.

Stefan Bräse will take us on “*A Trip to the Blue*”, highlighting how digital infrastructures can revolutionize the way chemists store, share, and analyse molecular data. Key initiatives include the **Molecule Archive**, a robust repository for the systematic capture and preservation of chemical knowledge; **Chemotion**, an open-source electronic lab notebook and repository platform; and **chemASAP**, a self-driving lab for organic synthesis analysis. Together, these tools create an integrated ecosystem that enhances collaboration, supports reproducibility, and accelerates the chemical innovation cycle.

Ute Schepers will present the role of **self-driving laboratories** in the accelerated discovery of novel materials for health applications. By combining automated synthesis, high-throughput screening, and machine-learning-driven decision-making, these platforms can explore vast chemical and biological spaces far beyond the reach of conventional methods. She will illustrate this through case studies on **peptoids** — versatile peptidomimetics with biomedical potential, biomaterials designed for advanced therapeutic functions, and AI-based applications for standardized 3D tissues and **organoids** as physiologically relevant 3D models for testing and validation.

Bringing these perspectives together, the lecture will explore how digital chemistry infrastructures and autonomous experimentation converge to form a powerful innovation pipeline — from molecular design to real-world biomedical solutions.