Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Institute for Molecular Physical Science (IMPS)

Einladung zu einem Kolloquium

Datum/Zeit:	**Dienstag, 18.02.2025, 16.45 Uhr**
Referent:	**Prof. Dr. Francesca Grisoni** Universität Eindhoven, Eindhoven, Netherlands
Titel:	*Exploring Chemical Space with AI in Low-Data Scenarios*
Ort:	**HCI G7**

The chemical universe is immensely vast – far beyond what can be experimentally explored. Efficiently navigating such chemical space is undoubtedly a daunting task, yet it holds immense potential for drug and materials discovery. Artificial intelligence (AI) has been gaining increasing attention in the molecular sciences, thanks to remarkable successes in fields such as computer vision, protein structure prediction, and natural language processing. However, in drug discovery and chemical biology, a major hurdle remains: the scarcity of known molecules with desirable properties. Such scarcity crucially limits the effectiveness of off-the-shelf AI approaches, which are usually data hungry. However, “everything’s not lost”, as several learning paradigms have the potential to overcome low-data limitations. This talk will reflect on the lessons learned, the challenges encountered, and the emerging opportunities in applying AI to low-data molecule discovery. It will also highlight successful strategies to address these challenges and facilitate the discovery of molecules with desirable properties – ranging from bioactivity prediction, supramolecular interaction elucidation, and de novo molecule design.

Gäste sind willkommen