Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Institute for Molecular Physical Science (IMPS)

Einladung zu einem Kolloquium

Datum/Zeit:	**Dienstag, 12.03.2024, 16.45 Uhr**
Referent:	**Prof. Prof. Stefan Vučković** University of Fribourg, Fribourg, Schweiz
Titel:	*Transforming DFT simulations for complex molecules*
Ort:	**HCI G7**

The accuracy of density functional approximations (DFAs) has become a limiting factor in scientific discoveries driven by electronic structure calculations and empowered by artificial intelligence. The development of DFAs is currently in "no man's land". On the one hand, machine-learned DFAs hold promise to overcome the known deficiencies of human-designed functionals. Yet, their transferability remains a major challenge, essential for the broad applicability seen in their traditional (human-designed) counterparts. In this talk, I will present our group's efforts in overcoming the long-standing deficiencies of traditional functionals and increasing the transferability of machine-learned functionals

Gäste sind willkommen