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in kemijsko tehnologijo

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

Dr. Marc Baaden

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z naslovom / title:

Game Engines & Metaverse: Immersive Technologies for Molecular Modeling

v sredo, 15. 11. 2023 ob 15. uri /
on Wednesday, 15. 11. 2023 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:

My team is dedicated to the study of complex molecular assemblies through interactive visualization, manipulation and analysis methods. We focus on molecular aggregation and assembly, in particular on the properties of supramolecular constructs in membrane environments. These molecular entities are dynamic by nature and embody complex shapes and interactions that require in-depth analysis.

The UnityMol framework, which is based on the Unity3D game engine, is at the center of our investigations. Our goal is to improve 3D contextual understanding through content-guided navigation, exploded views and semantic links between molecular objects and the corresponding analysis data. We have extended UnityMol's repertoire with specific visualizations for sugar molecules and electrostatic properties and integrated coarse-grained systems relevant for the simulation of membrane systems. These simplified visualizations are particularly suitable for interactive simulations, also in education or through crowdsourcing. These interactive simulations assist in the construction of molecules and enhance the hands-on learning experience.

An important aspect of our work is the integration of specialized hardware, including large, high-resolution screens, head-mounted virtual reality headsets and augmented reality setups. This focus on hardware integration underlines our commitment to pushing the boundaries of molecular modeling and making it an interactive and engaging subject to study.