

# Molecular Modeling with Schrödinger-Suite Workshop (ONLINE)

Mittwoch, 02. Dezember 2020 bis Donnerstag, 03. Dezember 2020 | 09:00 Uhr bis 16:00

Uhr

[Leibniz-Rechenzentrum \(LRZ\)](#) | 85748 Garching b. München, Boltzmannstr. 1

## Drug Discovery with Schrödinger Suite

The Schrödinger drug discovery platform encompasses solutions for predictive physics-based modeling, machine learning, data analytics, and collaboration. Through hands-on exercises and interactive presentations, we will work together with the attendees on industrial-level computational modelling tasks in the fields of chemical & biological molecular design. Beginning from target analysis and preparation of compound library via enumeration and virtual screening cascades involving ligand- and structure-based methodologies.

## Development and Discovery with Computational Materials Simulations

During this workshop, we will give an overview and hands-on training on the Schrödinger Materials Science Suite. We will particularly focus on efficient structure generation, automated workflows and property-oriented analysis tools, which are important to overcome challenges towards wider application of computational tools in the rational design of new materials in industry. We will discuss simulation approaches for different length and time scales, including quantum mechanics and molecular dynamics, as well as machine learning. The application areas and the level of complexity of the hands-on sessions will be tailored to the interests of the participants as stated in the registration form. Examples for possible focus areas could be, among others, polymers and soft matter, molecular reactivity and catalysis, organic electronics, solid-state materials, or machine learning. The final agenda and hands-on sessions will be announced closer to the event.

The final agenda and hands-on sessions (on Schrodinger Cluster) will be announced closer to the event.

Veranstalter:  
Leibniz-Rechenzentrum (LRZ)

Boltzmannstr. 1  
85748 Garching b. München

<https://www.lrz.de>

Weitere Informationen: [https://www.lrz.de/services/compute/courses/2020-12-02\\_hmms1w20/](https://www.lrz.de/services/compute/courses/2020-12-02_hmms1w20/)