Molecular and Materials Modeling

(with emphasis on hands-on-exercises on your own personal computer)

Hybrid course by

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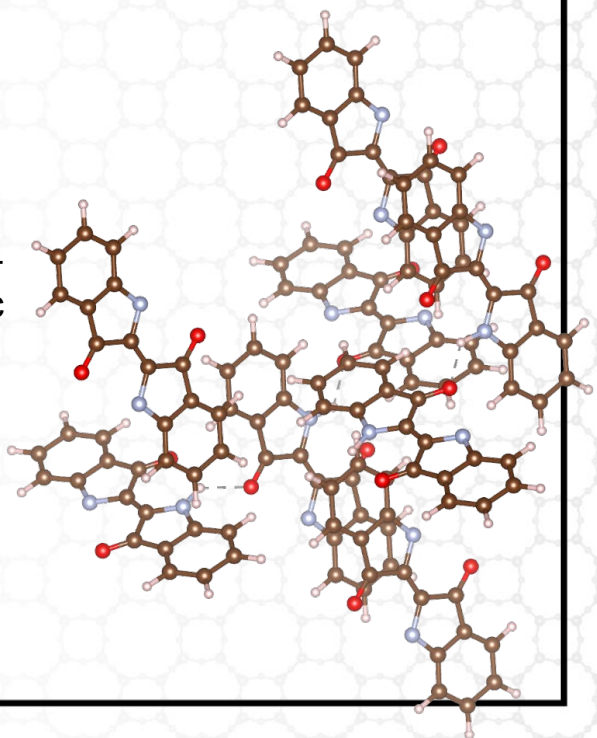
20. November 2026

Working with free/open source software on own computer ✔
Attendance in-person & via Zoom ✔
All lessons are recorded ✔
All working files are shared ✔

Atomic Simulation Environment (ASE)

Taste easy Python programming in ASE for molecular & material modeling.

Interatomic potentials - IPs (classic, machine learnt - MLIPs). Geometry optimization. Molecular and periodic systems. Adsorption on surfaces. Various.



Collaboration Opportunities with JINR

- For affiliated students, (co)tutoring BSc / MSc. / PhD. projects
- For affiliated students, participation in short-term JINR funded programs:
  International Students Practice (http://uc.jinr.ru/en/isp)
  START(https://start.jinr.ru/)
- For affiliated students, remote INTEREST programme (https://interest.jinr.ru/)
- Researchers from JINR member states and partner countries (https://www.jinr.ru/about-en/member-states-and-partners/) can be sent by their country for a research stay