Molecular and Materials Modeling

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

Hybrid course by

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15. May 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 (classic, reactive, machine learnt). Geometry optimization (local, global). Molecular and periodic systems. Adsorptions. Molecular dynamics. Various.


