Molecular and Materials Modeling

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

Online course by

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Working with free/open source software on own computer ✔
Connection via Zoom ✔
All lessons are recorded ✔
All working files are shared ✔

Part I: Molecular Modeling

Molecular mechanics & Quantum Mechanics - semiempirical, DFT, ab-initio
Geometry optimization; Electronic structure - atomic and molecular orbitals

Part II: Materials Modeling

Total energy calculation and geometry optimization
Electronic properties - density of states, band structure
Surfaces and 2D materials
Adsorption on surface

