

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 “0”: Own installation of computational apparatus

WSL-Ubuntu if MS Windows, or Linux operating system

Software: Avogadro, Jmol, VESTA, MOPAC, NWChem, ASE, Quantum ESPRESSO & all dependencies

Part I: Molecular Modeling

Molecular mechanics & Quantum Mechanics - semiempirical, DFT, ab-initio

Geometry optimization; Electronic structure - atomic and molecular orbitals

Spectroscopic, electric and magnetic properties

Solvent effects; excited states; reaction paths; Biomolecules

Part II: Materials Modeling

Periodic boundary condition - crystal symmetry and space group

Geometry optimization: variable cell vs. atomic relaxation

About supercells and surface slabs

Adsorption on surface: single atom,

Electronic and magnetic properties - density of states, band structure

Visualizing charge densities

