



Versatile Object-oriented Toolkit for Coarse graining and energy transport Applications

FAST. FLEXIBLE. FREE.
GROMACS

LAMMPS

ESPResSo++
Extensible Simulation Package for Research on Soft Matter

ESPResSo

VOTCA-CSG

- MD Topology Reader
- MD Trajectory Reader (**new: H5MD format**)
- Mapping of coordinates/forces
- Structure based coarse graining (**new: Iterative Integral Equation method**)
- Relative entropy
- Force matching

VOTCA-XTP

- DFT
- Many-Body Green's Function
- Bethe-Salpeter Equation
- Quantum classical embedding
- CUDA support
- OpenMP parallelization
- Python binding (**PyXTP**)

TOOLS

- Linear Algebra
- Wrappers

ASE

ORCA