Versatile **O**bject-oriented **T**oolkit for **C**oarse graining and energy transport **A**pplications

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