

VeloxChem

External
Libraries

SCF Optimization

Two-level DIIS

Spectroscopy

Response Theory

Generic Density
Matrix Construction

Numerical
Solvers

Python layer

Pybind11

C++ layer

Polarizable
Embedding

DFT
grid & weights
generation

Generic Kohn–Sham Matrix Construction

Integrals
Obara-Saika

DFT-kernel
Integration

