

GMSO

the General Molecular
Simulation Object

mBuild.Compound

parmed.Structure

Molecular Structure

SMILES

pdb

mol2

gro

lammps

Systematic and
Flexible Unit

Extensible
Workflow

Topology

Symbolic Potential
Expression

Molecular Topology File

CP2K

GOMC

GROMACS FAST.
FLEXIBLE.
FREE.

Cassandra
Monte Carlo
SOFTWARE

NAMD
Scalable Molecular Dynamics

hoomdblue

LAMMPS

Force Field Parameters

```
<?xml version='1.0' encoding='UTF-8'?>
<ForceField name="TIP3P" version="0.0.1">
  <FFMetaData>
    <Units energy="kJ/mol" mass="amu" charge="elementary_charge" distance="nm"/>
  </FFMetaData>
  <AtomTypes expression="4*epsilon * ((sigma/r)**12 - (sigma/r)**6)">
    <ParametersUnitDef parameter="epsilon" unit="kJ/mol"/>
    <ParametersUnitDef parameter="sigma" unit="nm"/>
    <AtomType name="opls_111" element="O" charge="-0.834" mass="16" definition="O"
description="water O">
      <Parameters>
        <Parameter name="epsilon" value="0.636586"/>
        <Parameter name="sigma" value="0.315061"/>
      </Parameters>
    </AtomType>
    <AtomType name="opls_112" element="H" charge="0.417" mass="1.011" definition="H">
      <Parameters>
        <Parameter name="epsilon" value="0.0"/>
        <Parameter name="sigma" value="1.0"/>
      </Parameters>
    </AtomType>
  </AtomTypes>
</ForceField>
```

MoSDeF

Molecular Simulation Design Framework