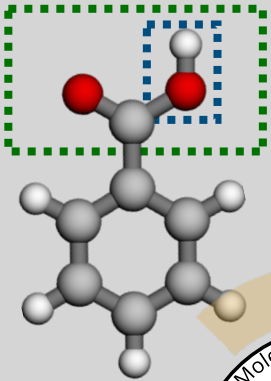
mBuild

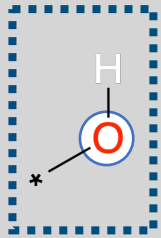
Construct your system

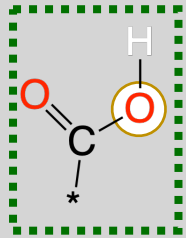
- Hierarchical system construction
- Create molecules
- Build complex systems
- Fill a simulation box
- And more!



Foyer

Define and apply your force field





Atom typing via SMARTS Matching

```
opls 154:
[O;X2]H
```

```
opls 268:
[O;X2]([C;%opls 267])H
overrides opls 154
```

- XML-based forcefields
- Robust overrides logic

Molecular Simulation MoSDeF Design Framework

Simulation Engines

Support for common MD and MC engines

HOOMD-blue

GOMC

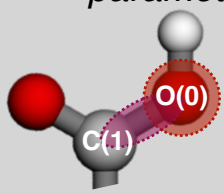
GROMACS FAST. FLEXIBLE. FREE.

LAMMPS

Cassandra Monte Carlo SOFTWARE

GMSO

View, edit, and save your parameterized system



- Supports arbitrary potential forms
- Parameters stored with units

Atom Types	
Index	O(0)
Type	opls 268
Sigma	3.0 Å
Charge	0.53 q

Bond Types	
Index	0
Atom1	O(0)
Atom2	C(1)
r_{eq}	1.364 Å