Select Atom

Input Unit Cell

Determine Edges
- Within scaled minimum distance
- Calculate RBF(d)
- $\leq N_{MAX}$ Hyperedges per atom

Determine Triplets
- All pairs of ovelapping edges
- Calculate RBF(Θ)
- $\leq N_{MAX} (N_{MAX} - 1)$ Hyperedges per atom

Determine Motif
- First shell (CrystalNN) of atoms
- Calculate CSMs, LSOPs
- 1 Hyperedge per atom