

Input Unit Cell

- distance
- Calculate RBF(d)
- $\leq N_{MAX}$  Hyperedges per atom
- edges
- Calculate  $RBF(\Theta)$
- $\bullet \le N_{MAX} (N_{MAX} 1)$ Hyperedges per atom
- of atoms
- Calculate CSMs, LSOPs
- 1 Hyperedge per atom

