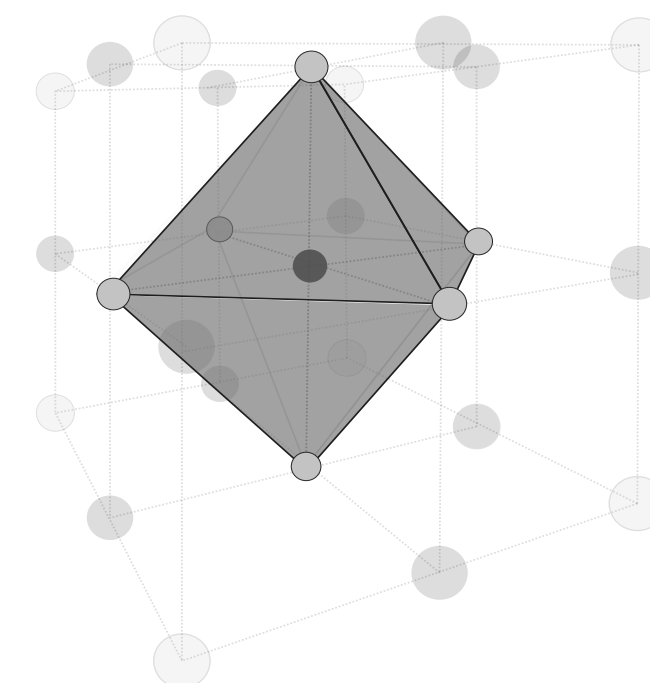
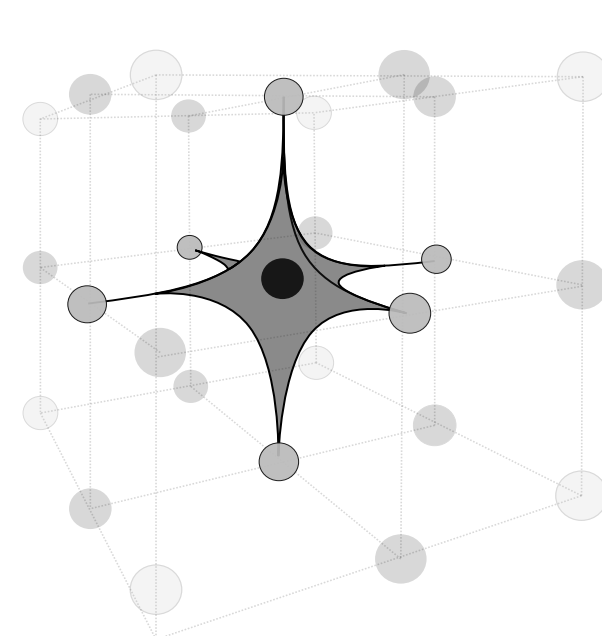
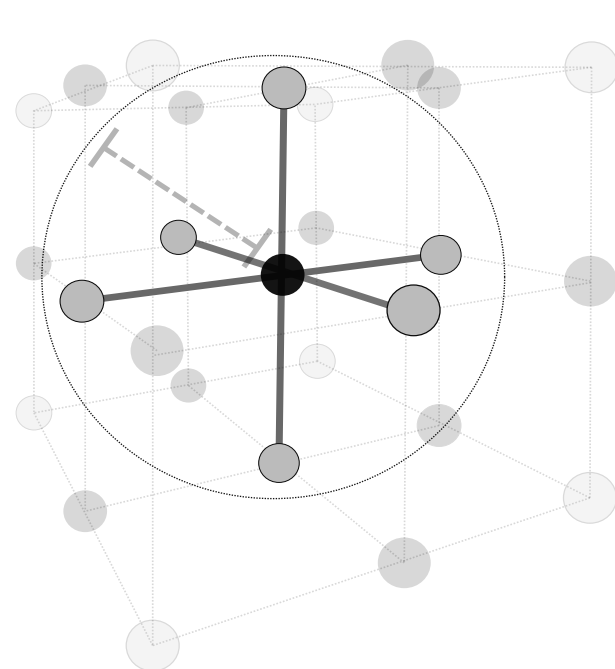
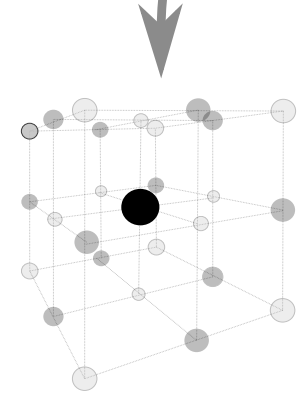


Select
Atom



Determine Edges

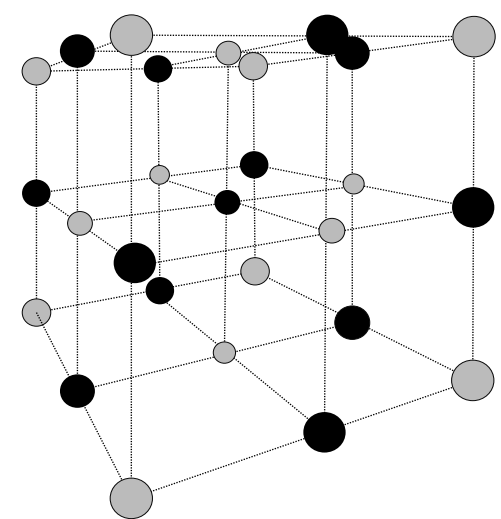
- Within scaled minimum distance
- Calculate $\text{RBF}(d)$
- $\leq N_{\text{MAX}}$ Hyperedges per atom

Determine Triplets

- All pairs of overlapping edges
- Calculate $\text{RBF}(\Theta)$
- $\leq N_{\text{MAX}} (N_{\text{MAX}} - 1)$ Hyperedges per atom

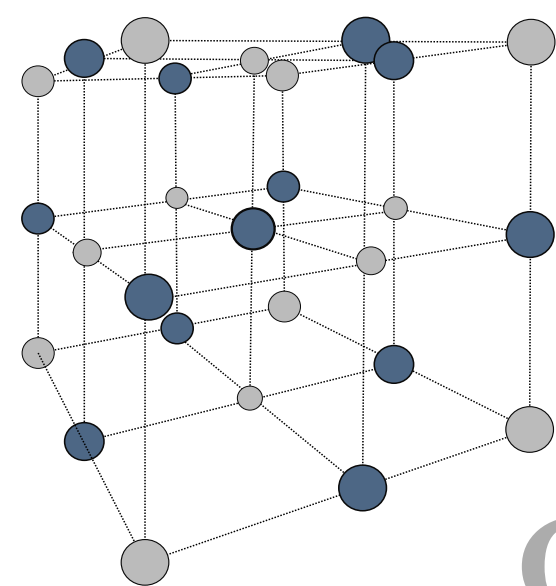
Determine Motif

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



Input Unit Cell

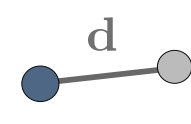
Ex:



C

6

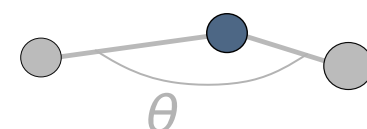
×



Bonds

15

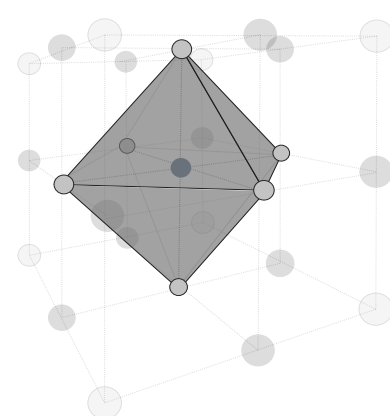
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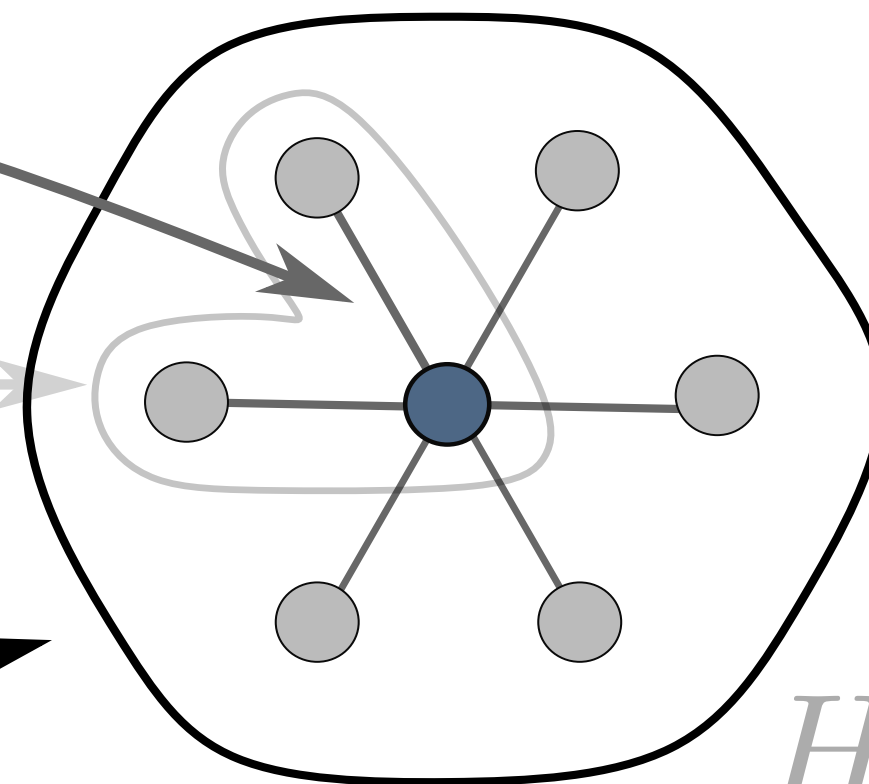
Triplets

1

×



Motif



$H(C)$