

Force Fields

1 Dual Lattice Force Fields

Currently, only one force field is implemented to optimise a structure's dual lattice. The total energy of a system is given by the sum of pair interaction energies:

$$\phi = \sum_{i=1}^{N_D} \sum_{j=i+1}^{N_D} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$