**Table S5** **The hyperparameters of training DP models.**

|  |  |  |
| --- | --- | --- |
| Hyperparameters | Symbols | DP model |
| cutoff radius |  |  |
| start learning rate |  | 0.001 |
| decay steps |  | 2000 |
| decay rate |  | 0.95 |
| energy initial prefactor |  | 0.02 |
| energy end prefactor |  | 2 |
| force initial prefactor |  | 1000 |
| force end prefactor |  | 1 |
| virial initial prefactor |  | 0.01 |
| virial end prefactor |  | 1 |
| smooth cutoff |  | 7.65 |
| embedding space dimension |  | 128 |
| training steps |  |  |