**Table S1** **The initial datasets.**

|  |  |
| --- | --- |
| Structures | The number of the initial datasets |
| Pt HCP | 40 |
| Pt FCC | 40 |
| Pt BCC | 40 |
| Pressure-perturbed Pt -  AIMD simulation samples | 150 (20 fs simulation at 50K) |