**Table S1 The parameters of AIMD simulations.**

|  |  |
| --- | --- |
| Quantities | Values |
|  | 50,300,500,700,900 |
| time step (fs) | 2 |
| simulation period (fs) | 20 |
| energy-cut-off (eV) | 1400 |
| -point mesh | 0.14 |
| EDIFF (eV) |  |
| ensemble |  |