|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Structure** | **Iterations** | **Cell size** | **No. of paths**  **(N\_legs)** | **Maximal displacement**  **(Å)** | **S02** | **dE0** |
| AIMD Ge-O-Ge 120° | 30000 | 3x3x3 | 4 | 0.4 | 0.9 | 0.5 |
| AIMD Ge-O-Ge 120° | 30000 | 3x3x3 | **2** | 0.4 | 0.9 | 0.5 |
| AIMD Ge-O-Ge 120° | 30000 | 3x3x3 | 4 | **0.35** | 0.9 | 0.5 |
| XRD Ge-O-Ge 120° | 30000 | 3x3x3 | 4 | **0.3** | 0.9 | 0.5 |
| AIMD Ge-O-Ge 120° | 30000 | 3x3x3 | 4 | **0.45** | 0.9 | 0.5 |
| AIMD Ge-O-Ge 120° | **15000** | 3x3x3 | 4 | 0.4 | 0.9 | 0.5 |
| **XRD Ge-O-Ge 130°** | 30000 | 3x3x3 | 4 | 0.4 | 0.9 | 0.5 |
| AIMD Ge-O-Ge 120° | 30000 | **4x4x4** | 4 | 0.4 | 0.9 | 0.5 |
| AIMD Ge-O-Ge 120° | 30000 | 3x3x3 | 4 | 0.4 | **1.0** | **0.0** |
| AIMD Ge-O-Ge 120° | **1** | 3x3x3 | 4 | 0.4 | 0.9 | 0.5 |
| **XRD Ge-O-Ge 130°** | **1** | 3x3x3 | 4 | 0.4 | 0.9 | 0.5 |