

- Systems:  $\text{Al}_{500}$  (1120 K),  $\text{C}_{512}$  (315.8 K),  $\text{Al}_{1372}$  (1120 K) and  $\text{He}_{2000}$  (2400 K).
- Exchange-correlation: PBE.
- Brillouin zone integration:  $\Gamma$ -point.
- Type of calculation: AIMD.
- Timestep: 1 fs ( $\text{Al}_{500}$ ,  $\text{Al}_{1372}$ ), 1.5 fs ( $\text{C}_{512}$ ) and 0.2 fs ( $\text{He}_{2000}$ ).
- Discretization: 0.66 Bohr ( $\text{Al}_{500}$ ,  $\text{Al}_{1372}$ ) and 0.3 Bohr ( $\text{C}_{512}$ ,  $\text{He}_{2000}$ ).
- Accuracy:  $\sim 1 \times 10^{-3}$  Ha/Bohr in force.