

- Systems: Bi_{32} and Cs_{29} slabs; Al_{256} and C_{216} bulk.
- Exchange-correlation: PBE.
- Brillouin zone integration: 4×4 grid (Bi_{32} and Cs_{29}); Γ -point (Al_{256} and C_{216}).
- Type of calculation: Single point.
- Discretization: 0.34 Bohr (Bi_{32}), 0.42 Bohr (Cs_{29}), 0.40 Bohr (Al_{256}), 0.25 Bohr (C_{216}).
- Accuracy: $\sim 1 \times 10^{-4}$ Ha/atom in energy.