- Systems: Au_{72} wire, C_{254} bilayer graphene, $(NiC_2O_4)_{54}$ bulk and $(TiO_2)_{32}$ slab. C_{254} and $(NiC_2O_4)_{54}$ have two vacancies.
- Exchange-correlation: PBE (Au_{72}), vdW-DF1 (C_{254}), SCAN ($(NiC_2O_4)_{54}$), HSE06 ($(TiO_2)_{32}$).
- Brillouin zone integration: 4 grid points (Au_{72}); Γ-point (C_{254},$(NiC_2O_4)_{54}$); 2×2 grid points ($(TiO_2)_{32}$).
- Type of calculation: Single point. Spin-polarized (C_{254}, $(NiC_2O_4)_{54}$).
- Discretization: 0.25 Bohr (Au_{72}, $(TiO_2)_{32}$), 0.29 Bohr (C_{254}), 0.24 Bohr ($(NiC_2O_4)_{54}$) in SPARC; 40 Ha (Au_{72}, C_{254}, $(TiO_2)_{32}$), 50 Ha ($(NiC_2O_4)_{54}$) in QE.
- Accuracy: $\sim 1 \times 10^{-4}$ Ha/atom in energy.