



Figure S1. Convergence tests for MgAgF₃ at 0 GPa.

Convergence of the total energy with respect to (a) the plane-wave cutoff energy and (b) the **k**-point mesh, plotted as the energy difference ΔE relative to the chosen parameters (570 eV and $3 \times 3 \times 1$ mesh, respectively). The horizontal dashed line at $\Delta E = 0$ indicates the reference value. In (a), the energy difference decreases rapidly above 500 eV, with $\Delta E = 0.021$ eV at 550 eV and less than 0.025 eV for all cutoffs above 570 eV. In (b), increasing the **k**-point mesh from $3 \times 3 \times 1$ to $4 \times 4 \times 1$ changes the energy by only 0.0016 eV, confirming that the chosen parameters are well converged.