

Supplementary material

In this study, convergence tests were conducted on the Cr_4AlB_4 . The results of the tests are presented in Fig.S1. To achieve convergence, a cutoff energy of 750 eV or more and a k-point mesh separation of less than 0.03 \AA^{-1} were necessary. During the convergence test on Encut, the K-space was set to 0.04 1/\AA . The convergence test on K-space was performed using an Encut of 750 eV.

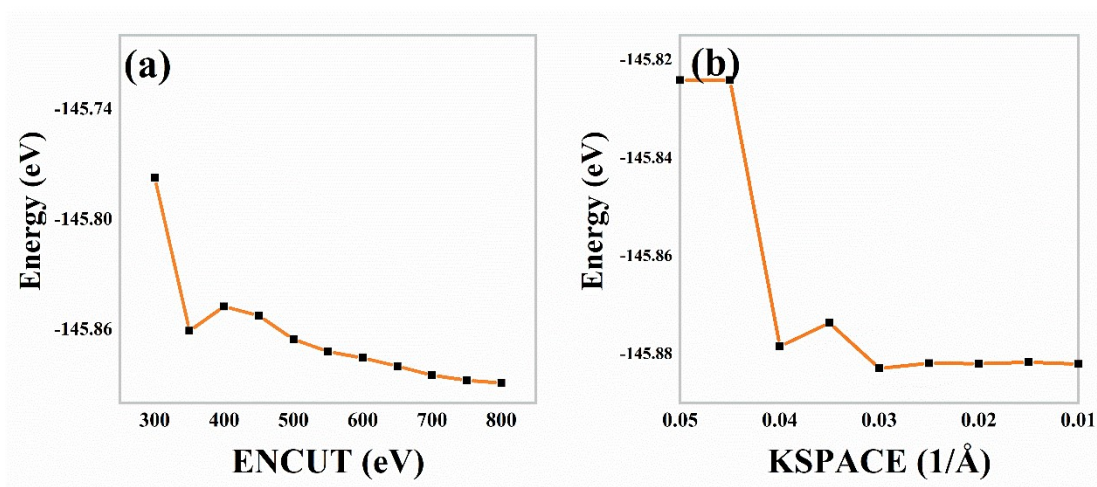


Fig.S1 Convergence test results for (a) Encut and (b) K-space