Electronic Supplementary Material (ESI) for Nanoscale. This journal is © The Royal Society of Chemistry 2019 Figure 1. Phonon band structures of MAB phases.









































Wave vector





Wave vector

Wave vector







Mo₄AlB₆













0

Wave vector

The instability of various MAB phases with respect to the type of transition metal.

FC_M (eVÅ⁻²)

The summation of force constants of all springs connected to an M atom in MAB phases with respect to the type of transition metal.

FC_{AI} (eVÅ⁻²)

FC_B (eVÅ⁻²)

Exfoliation energy (eVÅ⁻²)

Exfoliation energies of MAB phases with respect to the type of transition metal.

The data in Figure 3(a) are presented for each phase separately

 M_2AIB_2

 $M_3Al_2B_2$

 M_3AIB_4

atom-atom distance (Å)

 M_4AIB_6

MAIB

The data in Figure 3(b) are presented for each phase separately

M₄AIB₆

MAIB

The data in Figure 4(a) are presented for each phase separately

 M_2AIB_2

 M_4AIB_6

MAIB

The data in Figure 4(b) are presented for each phase separately

E_{exf} (eVÅ⁻²)

0.16

0.18

0.2

0.22

0.14

20 └─ 0.08

0.1

0.12

