

3
4
Cr Ti Al C
1.5 1.5 1 1.9
1
1724
2 1 1 2
-103
2
6
0

INPUT

Row	Data Type // Physical Significance and Notes
line 1	int // select program function; 1 for obtaining Gibbs free energy, 2 for analyzing synthesis prospect, 3 for predicting impurities
line 2	int // the number of element types
line 3	char // the elements
line 4	double // the starting element ratio; shall be the standard stoichiometric ratio when line 1 is 2
line 5	int // the type of target MAX phase; 1, 2, 3 and 4 represent o-MAX, solid solution, i-MAX and conventional MAX structure respectively
line 6	double // temperature; have to be an even number
line 7	double // the standard stoichiometric ratio of the target MAX phase
line 8	float // ground state energy from DFT calculation (eV/cell)
line 9	int // number of copies of the chemical formula contained in the unit cell
line 10	double // total number of transition metal atoms in the unit cell
line 11	double // solid solution concentration of M atom; specify 0 for crystal structure
*** Not all lines are required. When the 1 function is selected, line1-7 can be blank and input conditions should be specified directly from line 8; When the 2 or 3 function is selected, line8-11 can be blank.	