First principles study on stability and hydrogen adsorption properties of Mg/Ti interface

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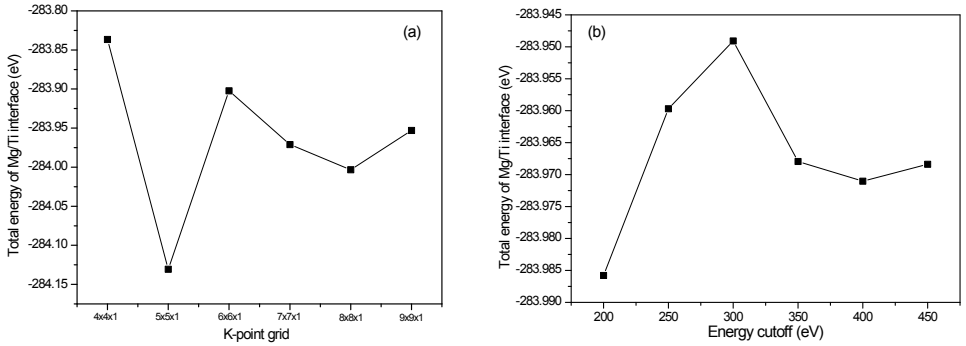
Supporting Information: Calculation Details

Fig. S1 The detailed tests about the dependence of total energy of Mg/Ti interface on (a) the k-point grids and (b) energy cutoff for a (2×2) slab model.



It can be seen that variation of three points in Fig. S1(a) is within 0.0001% related to the absolute value of the total energy. Therefore the 7x7x1 k-points were used. In Fig. S1(b), after 350 eV, the dependence of total energy on the energy cutoff is weak, and the value of 400 eV was employed.

Table S1 The adsorption sites (in fraction coordinates) of hydrogen in the interface model.

H positions	*u*	*v*	*w*
bridge	0.417	0.833	0.315
fcc	0.500	0.500	0.315
hcp	0.333	0.667	0.315
top	0.167	0.833	0.315
Mg-tet1	0.333	0.667	0.352
Mg-tet2	0.667	0.333	0.377
Mg-oct	0.500	0.500	0.364
Ti-tet1	0.333	0.667	0.260
Ti-tet2	0.667	0.333	0.280
Ti-oct	0.500	0.500	0.270

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