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Supporting information

First-principles investigation of the hydrogen evolution reaction of transition metal phosphides CrP, MnP, FeP, CoP, and NiP

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Computational details

We performed first-principles calculation to investigate the hydrogen evolution reaction of CrP, MnP, FeP, CoP, and NiP. The structures were fully relaxed, and the obtained lattice constants were listed in the following table 1.

Table 1: Lattice constants of considered MP.

	a (Å)	b (Å)	c (Å)
CrP	5.908	5.288	3.029
MnP	5.820	5.156	3.098
FeP	5.109	5.712	3.003
CoP	5.519	5.022	3.219
NiP	5.808	4.868	3.408

For the surface calculations, we used 6 layers of atoms for the surface models (see Fig. 1, and we fixed the bottom 4 layers. We considered various adsorption sites for the hydrogen adsorption on the surface. Those adsorption sites were shown in the following Fig. 1, including the sites on top of the metal atoms with different coordination (denoted as T_{M1} and T_{M2}), and the bridge sites between two atoms, for example, between the two metal atoms M_1 and M_2 (denonted as $B_{M1-M1'}$) or between the metal atom and phosphorus atom (denonted as B_{M1-P1} or B_{M1-P2})

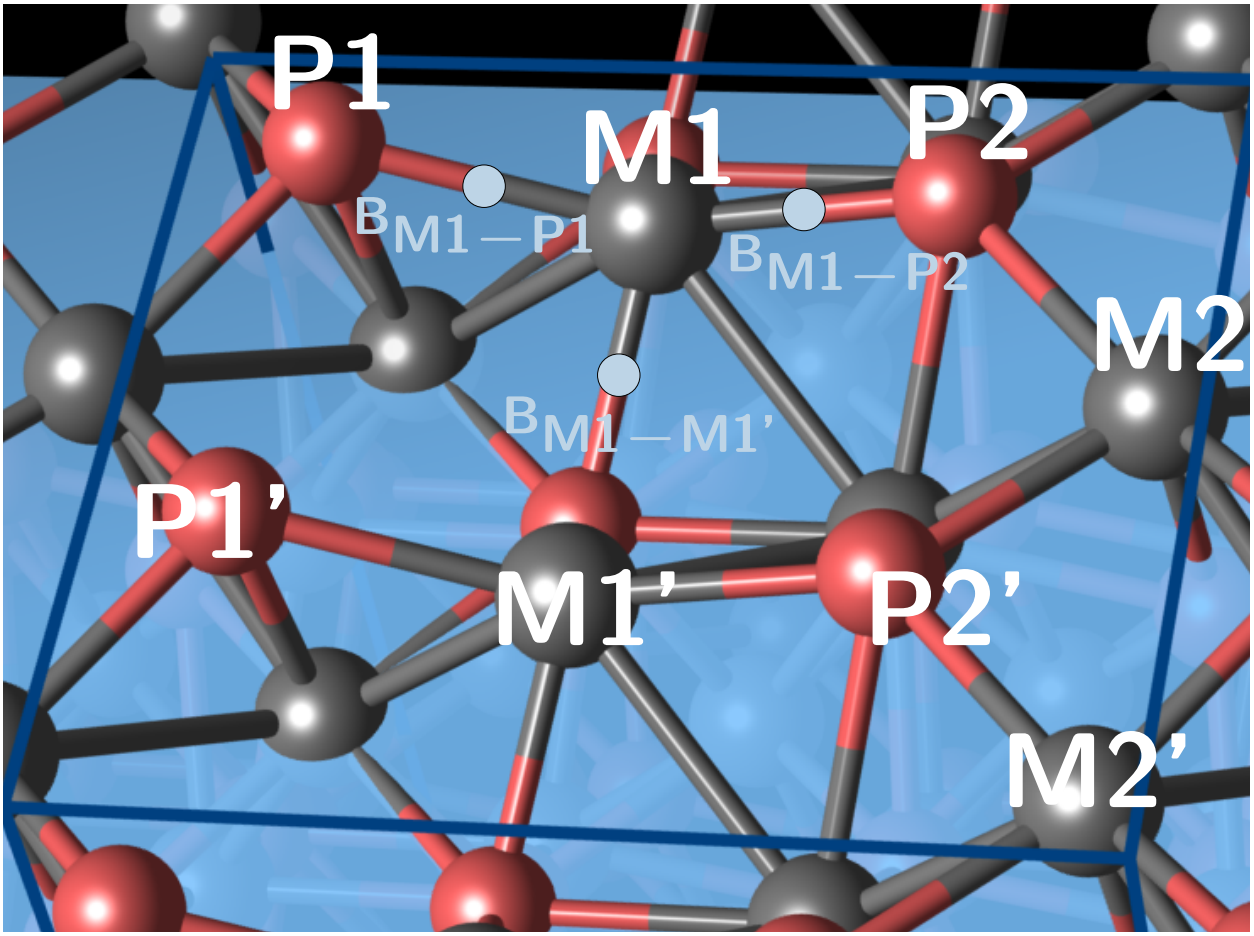

Figure 1: The adsorption sites on the surface. The dark blue line is the cell boundary.