Supplementary Information: Hydrogen adsorption trends on Al-doped Ni$_2$P surfaces for optimal catalyst design

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1 H-adsorption energies for Ni$_3$P$_2$ termination of Ni$_2$P

Optimised hydrogen adsorption energies for the first (green triangle) and second (purple square) hydrogens at the 14 investigated hydrogen starting positions (H identifier) on top of the Ni$_3$P$_2$ terminated Ni$_2$P slab. The dashed black line indicates the $\Delta G_H$ of the first hydrogen adsorption for the pristine slab, whereas the dashed red line shows the second hydrogen adsorption $\Delta G_H$ value for the pristine slab. As described in the article, the deep yellow band highlights the $\pm$0.1 eV region around the optimal $\Delta G_H = 0$ value. For example, in Figure S1, the green triangle at H identifier 13 corresponds to the black triangle at Mg (l1d1) in Figure 5 of the main article. Similarly, the purple square at H identifier 1 corresponds to the green square at Mg (l1d1) in the same Figure.
1.1 Dopants on a single layer

Figure S1: Mg (l1d1)

Figure S2: Mg (l2d1)
Figure S3: Mg (l2d3)

Figure S4: V (l2d1)
Figure S5: V (l2d3)

Figure S6: V (l3d1)

S4
Figure S7: V (l4d1)

Figure S8: Fe (l2d2)
Figure S9: Fe (l3d1)

Figure S10: Fe (l3d2)
Figure S11: Co (11d2)

Figure S12: Co (12d1)
Figure S13: Co (l3d2)

Figure S14: Cu (l1d1)
Figure S15: Mo (l1d1)

Figure S16: Mo (l2d1)
1.2 Dopants on two layers
Figure S19: Co (l1l3)

Figure S20: Mg (l2l4)
Figure S21: Cu (1112)

Figure S22: Cu (1113)
2 H-adsorption energies for Ni\textsubscript{3}P\textsubscript{2}+P termination of Ni\textsubscript{2}P

Optimised hydrogen adsorption energies for the first (green triangle), second (purple square), and third (red circle) hydrogens at the 14 investigated hydrogen starting positions on top of the Ni\textsubscript{3}P\textsubscript{2}+P terminated Ni\textsubscript{2}P slab. The dashed black line indicates the $\Delta G_\text{H}$ of the first hydrogen adsorption for the pristine slab, whereas the dashed red line shows the second hydrogen adsorption $\Delta G_\text{H}$ value for the pristine slab. As described in the article, the deep yellow band highlights the $\pm 0.1$ eV region around the optimal $\Delta G_\text{H} = 0$ value. For example, in Figure S23, the green triangle at H identifier 2 corresponds to the black triangle at Mg (l1d1) in Figure 7 of the main article. Similarly, the purple square at H identifier 12 corresponds to the green square at Mg (l1d1) in the same Figure.

2.1 Dopants on a single layer

Figure S23: Mg (l1d1)
Figure S24: Mg (l1d3)

Figure S25: Mg (l2d2)
Figure S26: V (l1d1)

Figure S27: V (l2d1)
Figure S28: V (l2d2)

Figure S29: V (l4d1)
Figure S30: Fe (11d1)

Figure S31: Fe (11d2)
Figure S32: Fe (11d3)

Figure S33: Fe (13d2)
Figure S34: Co (11d1)

Figure S35: Co (12d2)
Figure S36: Co (l3d1)

Figure S37: Cu (l2d1)
Figure S38: Mo (l1d1)

Figure S39: Mo (l2d1)
Figure S40: Mo (l2d3)

Figure S41: Mo (l3d3)
2.2 Dopants on two layers

Figure S42: Co (1112)