Supplementary Information

Theoretical proposal of a revolutionary water-splitting photocatalyst:

The monolayer of boron phosphide

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TABLE I. Calculated results: Gibbs free energy G, total energy calculated by DFT E^{DFT}, zero-point energy calculated by DFT E^{ZPE}, enthalpy change $\Delta H^{\circ}(0\mathrm{K} \rightarrow T)$, standard entropy S°, and Gibbs free energy at standard conditions G°. The unit is eV.

	G	E^{DFT}	E^{ZPE}	$\Delta H^{\circ}(0\mathrm{K} \rightarrow T)$	$-T\,S^{\circ}$	G°
*		-49.059				
O*	-6.392	-55.545	0.094			
OH*	-9.902	-59.335	0.374			
OOH*	-15.877	-65.375	0.439			
H*0	-2.555	-51.850	0.235			
H*1	-2.702	-58.494	0.247			
H*2	-3.860	-63.427	0.232			
H*3	-4.322	-69.940	0.243			
H_2(g)	-6.827	-6.771	0.271	0.088	-0.404	-6.816
H_2O(g)		-14.219	0.572	0.103	-0.584	-14.128
H_2O(l)	-14.216					-14.216
O_2(g)	-9.911					-9.883
$H^+ + e^-$	$-3.408 - 0.0592\,pH + V_{\mathrm{e}}$					-3.408

TABLE II. The change of Gibbs free energy ΔG, and overpotentials η_{HER} and η_{OER} along each pathway. The unit is eV.

HER pathways

(a) $H^+ + e^- + * \rightarrow H*0$	$\Delta G = 0.853 + 0.0592\,pH - V_e$	$\eta_{\mathrm{HER}} = 0.858$
(b) $H^+ + e^- + H*0 \rightarrow H_2(g) + *$	$\Delta G = -0.863 + 0.0592\,pH - V_e$	$\eta_{\mathrm{HER}} = -0.858$
(c) $2\,H*0 \rightarrow H_2(g) + 2\,*$.	$\Delta G = -1.716$	
(a) $H^+ + e^- + * \rightarrow H*1$	$\Delta G = 0.706 + 0.0592\,pH - V_e$	$\eta_{\mathrm{HER}} = 0.711$
(b) $H^+ + e^- + H*1 \rightarrow H_2(g) + *$	$\Delta G = -0.717 + 0.0592\,pH - V_e$	$\eta_{\mathrm{HER}} = -0.711$
(c) $2\,H*1 \rightarrow H_2(g) + 2\,*$.	$\Delta G = -1.423$	
(a) $H^+ + e^- + * \rightarrow H*2$	$\Delta G = -0.452 + 0.0592\,pH - V_e$	$\eta_{\mathrm{HER}} = -0.447$
(b) $H^+ + e^- + H*2 \rightarrow H_2(g) + *$	$\Delta G = 0.441 + 0.0592\,pH - V_e$	$\eta_{\mathrm{HER}} = 0.447$
(c) $2\,H*2 \rightarrow H_2(g) + 2\,*$.	$\Delta G = 0.893$	
(a) $H^+ + e^- + * \rightarrow H*3$	$\Delta G = -0.914 + 0.0592\,pH - V_e$	$\eta_{\mathrm{HER}} = -0.909$
(b) $H^+ + e^- + H*3 \rightarrow H_2(g) + *$	$\Delta G = 0.904 + 0.0592\,pH - V_e$	$\eta_{\mathrm{HER}} = 0.909$
(c) $2\,H*3 \rightarrow H_2(g) + 2\,*$.	$\Delta G = 1.818$	

OER pathways

(d) $H_2O(l) + * \rightarrow OH* + H^+ + e^-$	$\Delta G = 0.906 - 0.0592\,pH + V_e$	$\eta_{\mathrm{OER}} = -0.316$
(e) $OH* \rightarrow O* + H^+ + e^-$	$\Delta G = 0.102 - 0.0592\,pH + V_e$	$\eta_{\mathrm{OER}} = -1.120$
(f) $2\,OH* \rightarrow H_2O(l) + O* + *$	$\Delta G = -0.804$	
(g) $H_2O(l) + O* \rightarrow OOH* + H^+ + e^-$	$\Delta G = 1.323 - 0.0592\,pH + V_e$	$\eta_{\mathrm{OER}} = 0.101$
(h) $OOH* \rightarrow O_2(g) + * + H^+ + e^-$	$\Delta G = 2.558 - 0.0592\,pH + V_e$	$\eta_{\mathrm{OER}} = 1.336$
(i) $2\,OOH* \rightarrow O_2(g) + 2\,O* + 2\,H^+ + 2\,e^-$	$\Delta G = 2.242 + 2(-0.0592\,pH + V_e)$	$\eta_{\mathrm{OER}} = -0.101$