Support information

New Insight on Hydrogen Evolution Reaction Activity of MoP_2 from Theoretical Perspective

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Table S1. Adsorption energy of the optimized hydrogen adsorption sites for (111) facet. (unit in eV)

Adsorption sites	Mo1	P1	Mo2	P2	Mo1-P2	Mo1-P3
111-facet	-0.106	-0.038	0.083	0.402	0.251	0.016

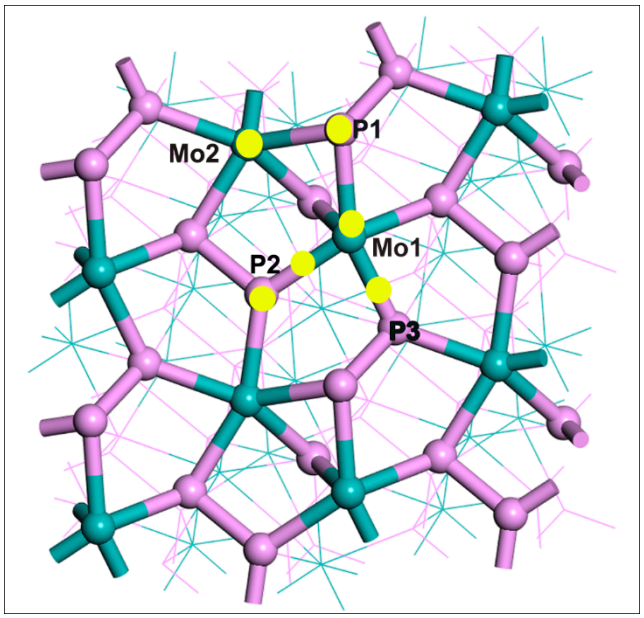

Figure S1. All possible adsorption sites on (111) facet.

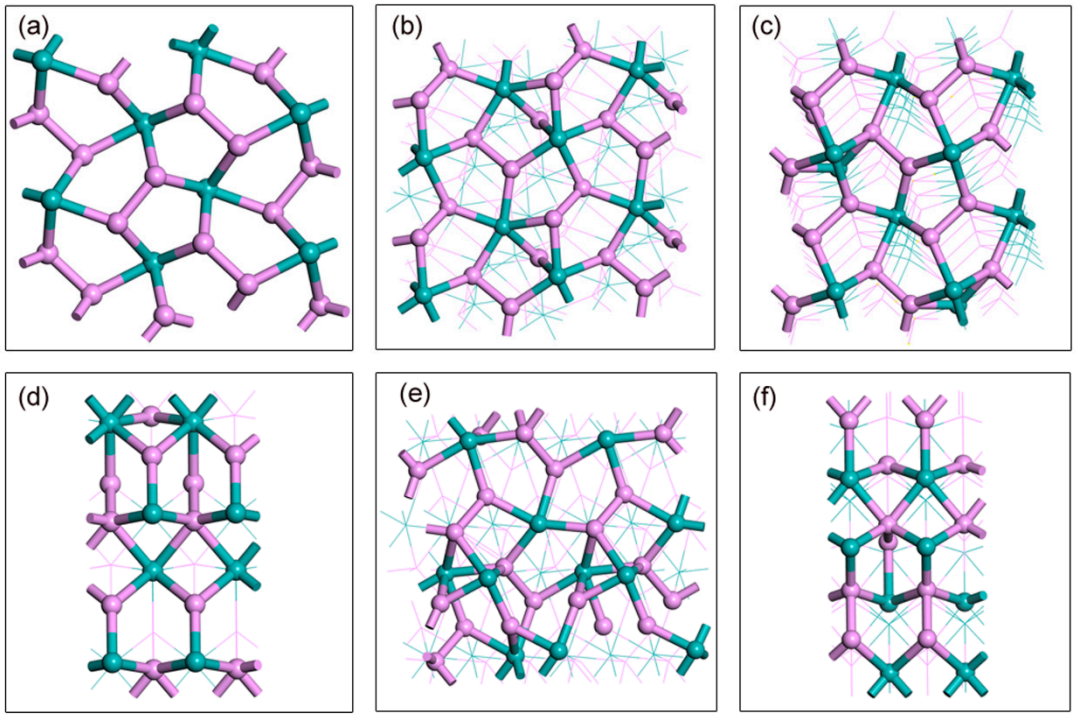

Figure S2. Top view of six clean MoP_2 surfaces, including (a) (100), (b) (111), (c) (110), (d) (001), (e) (101) and (f) (011) facets. Mo: dark green; P: purple.