Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for A Comprehensive Understanding of Water Photooxidation on Ag_3PO_4 Surfaces

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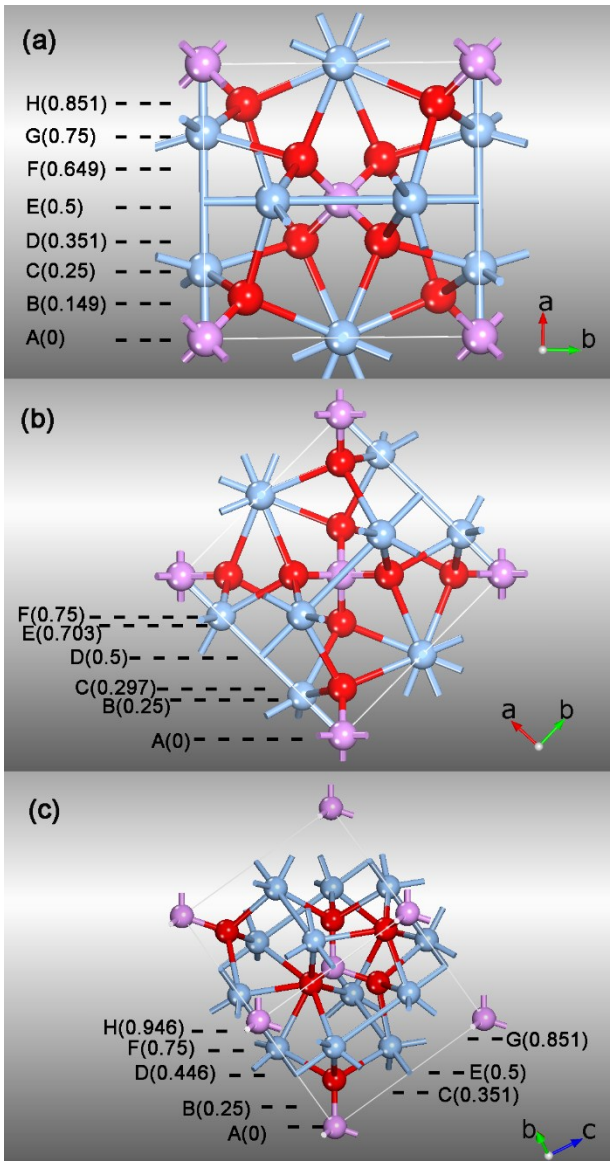

Fig.S1. The sliced terminations of a cubic Ag_3PO_4 crystal at vertical [100] (a), [110] (b), and [111] (c) direction.

Table S1. The total energies (E: eV) and formation energies (E_f : J/m^2) of surface-terminated models depicted in Fig.S1. The surface was modeled using a period slab with a vacuum space of 15 Å in the direction of surface normal and a thickness that contains six Ag_3PO_4 units.

100			110			111		
Top	E	E_f	Top	E	E_f	Top	E	E_f
A: 0	-244.660	1.917	A: 0	-246.974	1.002	A: 0	-248.254	0.659
B: 0.149	-251.957	0.341	B: 0.25	-244.867	1.324	B: 0.25	-246.903	0.827
C: 0.25	-251.961	0.340	C: 0.297	-251.064	0.3776	C: 0.351	-238.349	1.894
D: 0.351	-244.656	1.918	D: 0.5	-251.062	0.3779	D: 0.446	-240.662	1.605
E: 0.5	-244.656	1.918	E: 0.703	-244.866	1.324	E: 0.5	-248.2597	0.658
F: 0.649	-251.949	0.343	F: 0.75	-246.972	1.003	F: 0.75	-246.902	0.827
G: 0.75	-251.981	0.336				G: 0.851	-238.341	1.895
H: 0.851	-244.661	1.919				H: 0.946	-248.2598	0.658

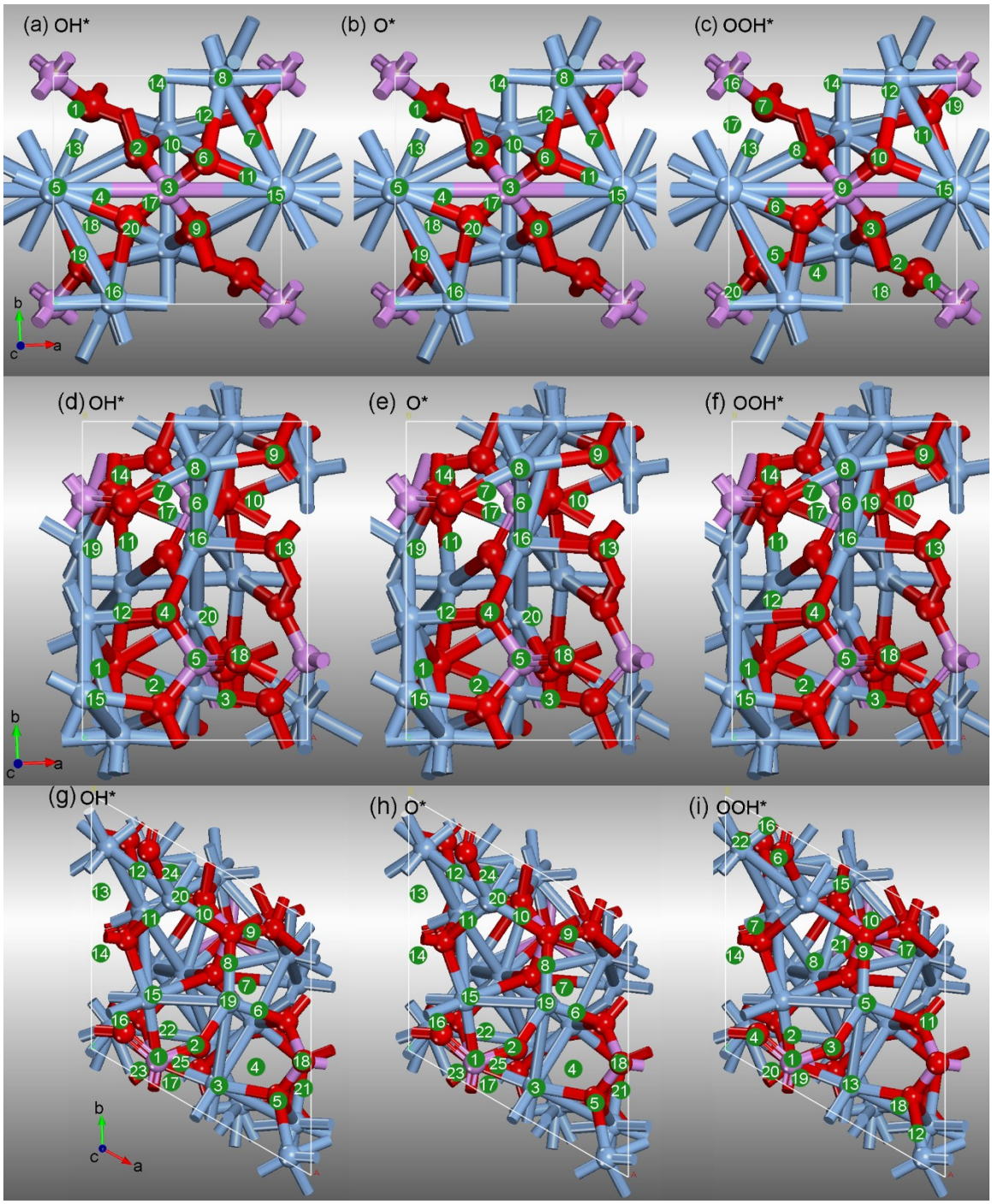

Fig.S2. The initial adsorption sites for relevant species (OH*, O* and OOH*) during OER on Ag_3PO_4 (100) (a-c), (110) (d-f) and (111) (g-i) surfaces.

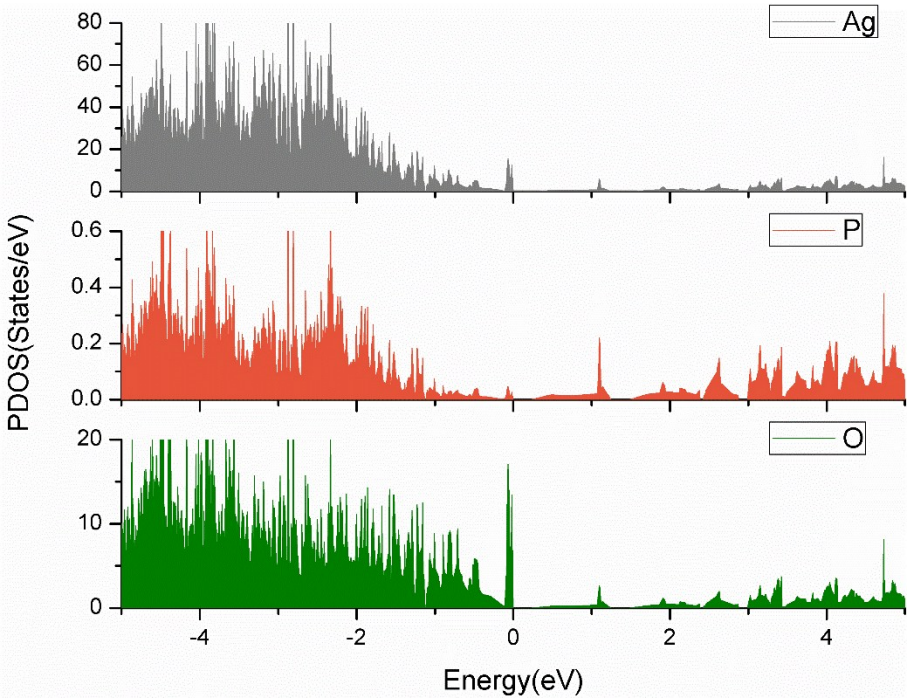

Fig.S3. Partial DOS of the Ag_3PO_4 (100) surface.

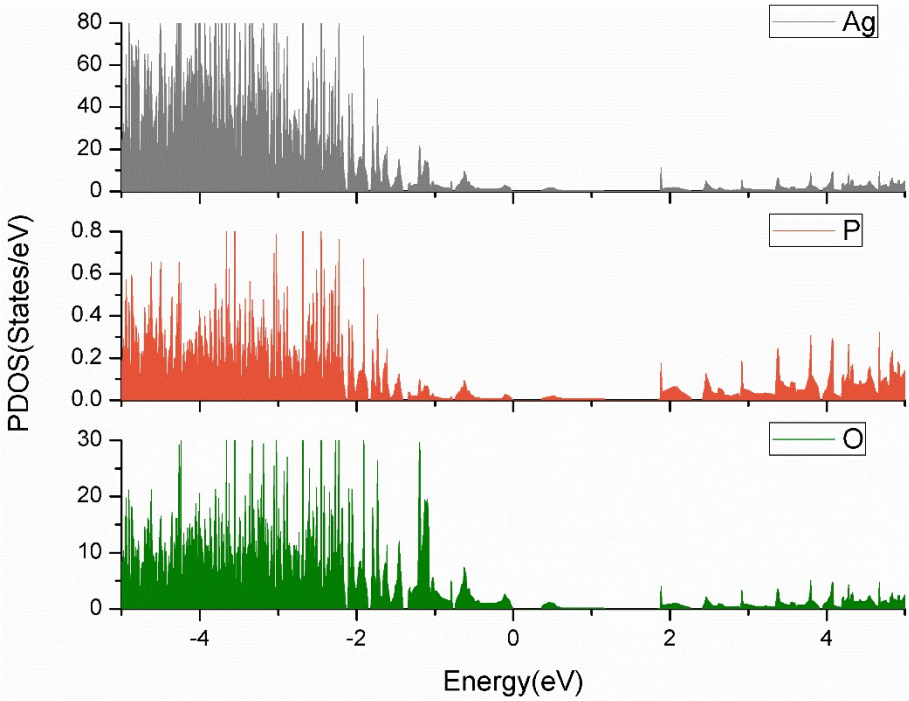

Fig.S4. Partial DOS of the Ag_3PO_4 (110) surface.

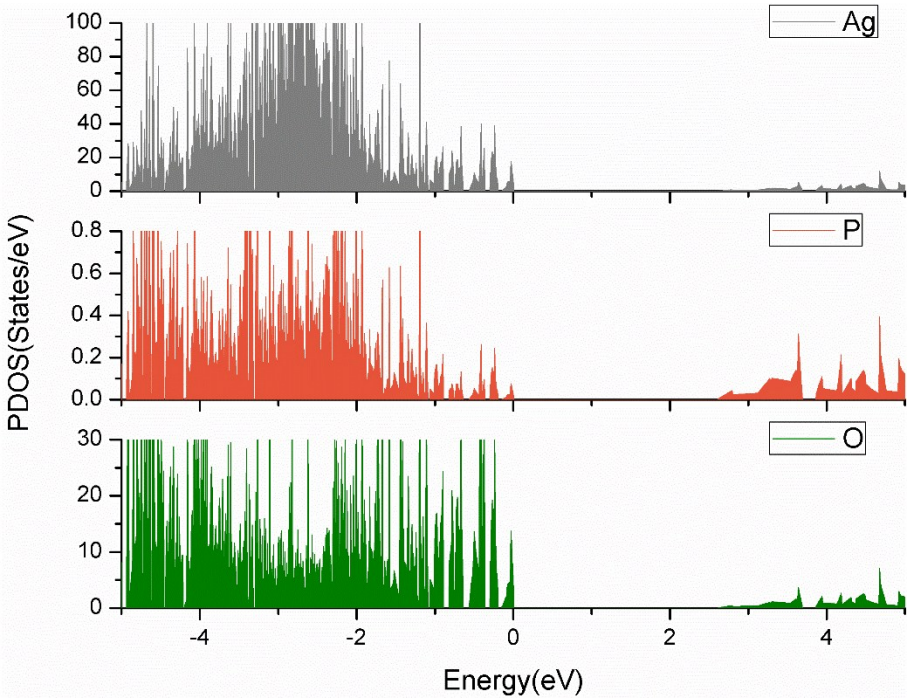

Fig.S5. Partial DOS of the Ag_3PO_4 (111) surface.

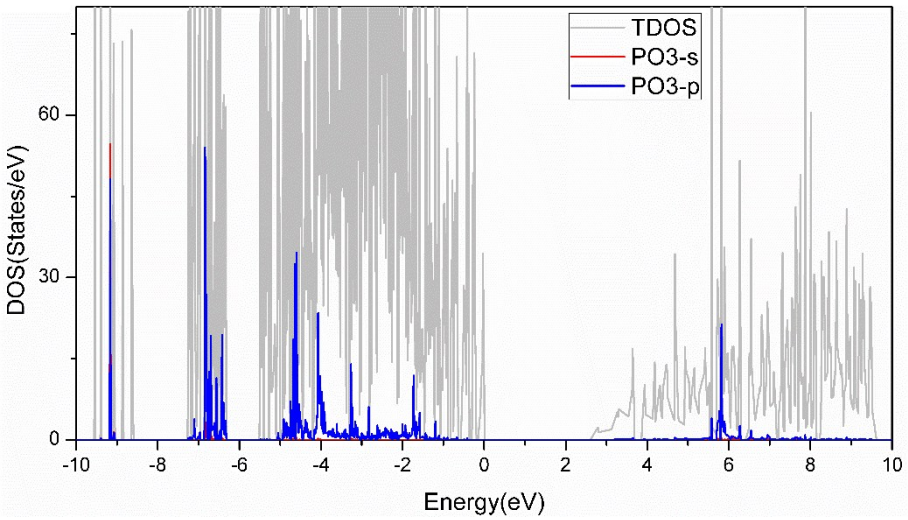

Fig. S6. Total DOS of (111) surface (TDOS) and partial DOS of [PO3] unit on the top layer of (111) surface

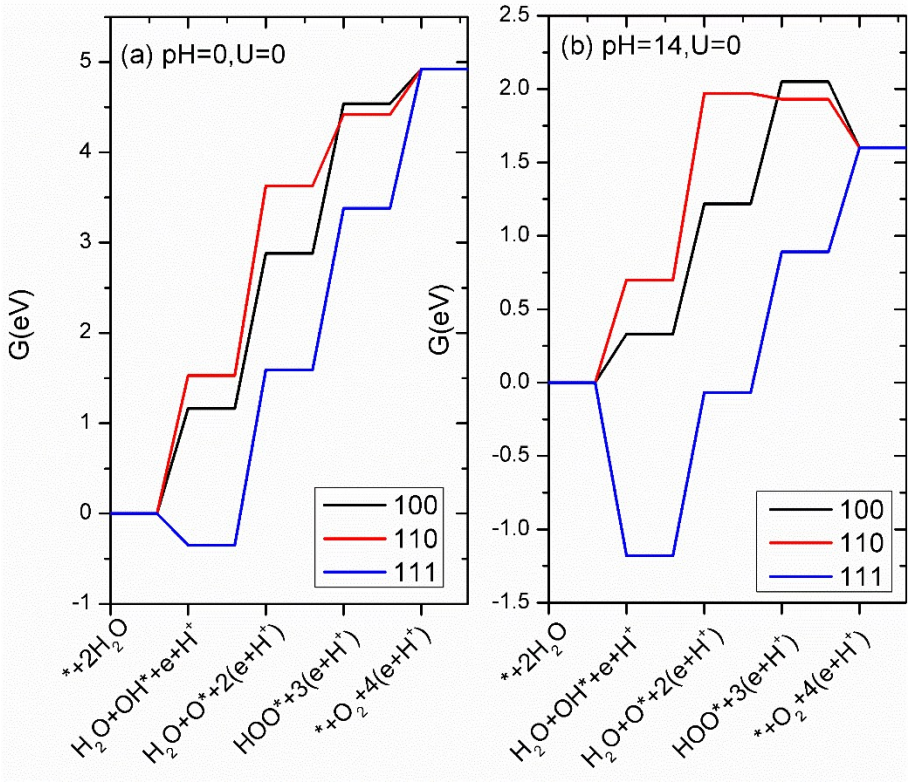

Fig. S7. The free energies of the intermediates on the Ag_3PO_4 surfaces following mechanism I at pH = 0 (a), and pH=14 (b).