Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2022

Supporting Information

Water oxidation mechanism of cobalt phosphate catalyst in artificial photosynthesis: a theoretical study

Takao Tsuneda[*,a,b] and Seiichiro L. Ten-no[a]

[a] Graduate School of Science Technology and Innovation, Kobe University, Nada-ku, Kobe, Hyogo 657-8501, Japan

[b]Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo 060-0810, Japan

* Corresponding author: tsuneda@phoenix.kobe-u.ac.jp

Fig. S1. Calculated vibrational spectrum of hydrated CoPi cluster model for the optimized reactant structure using the singlet-state cobalt-oxide surface in the singlet state. The curve at the top is the experimental infrared spectrum of CoPi surface, which is excerpted from Ref. 38 for comparison. The main vibrational spectral band assignment is also shown.

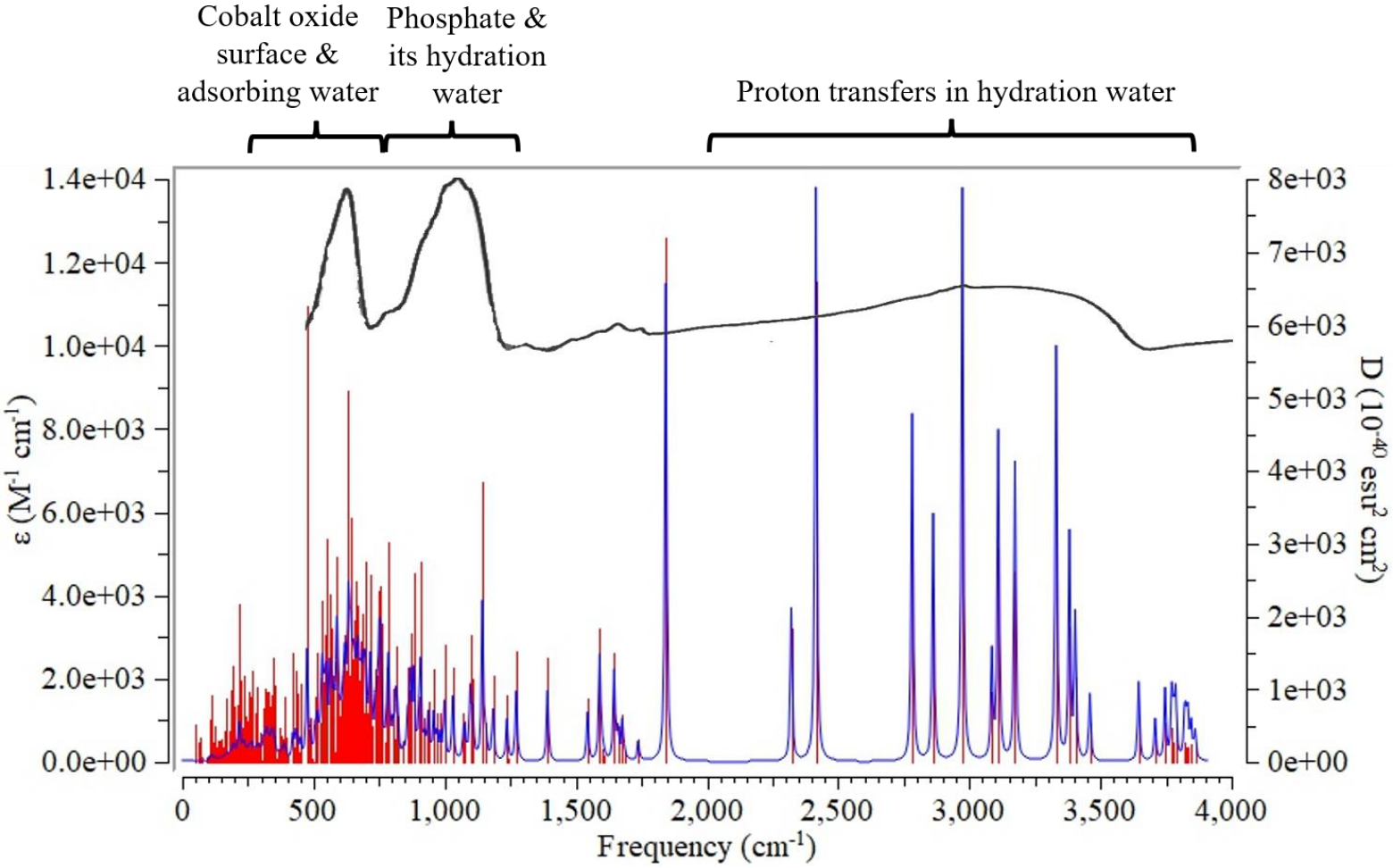

Fig. S2. The optimum geometries of the reactants in the water oxidation reaction mechanisms of hydrated CoPi surface with the (a) singlet- and (b) doublet-state cobalt oxide surfaces for the singlet (left) and triplet (right) states.

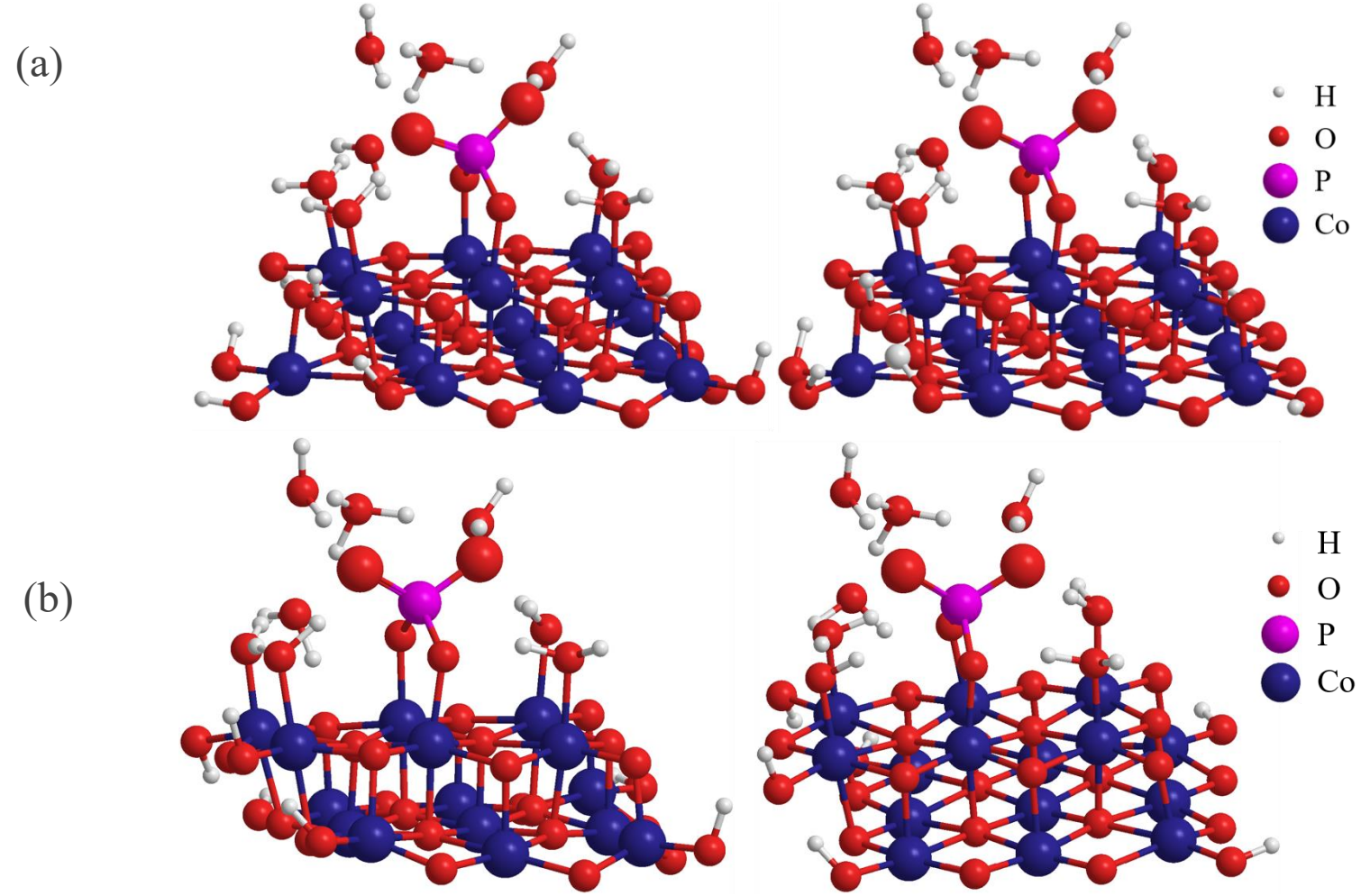

Fig. S3. Water oxidation reaction mechanism of hydrated CoPi surface in the triplet state for the doublet-state cobalt oxide surface. Formed O-O bonds are indicated in green circles.

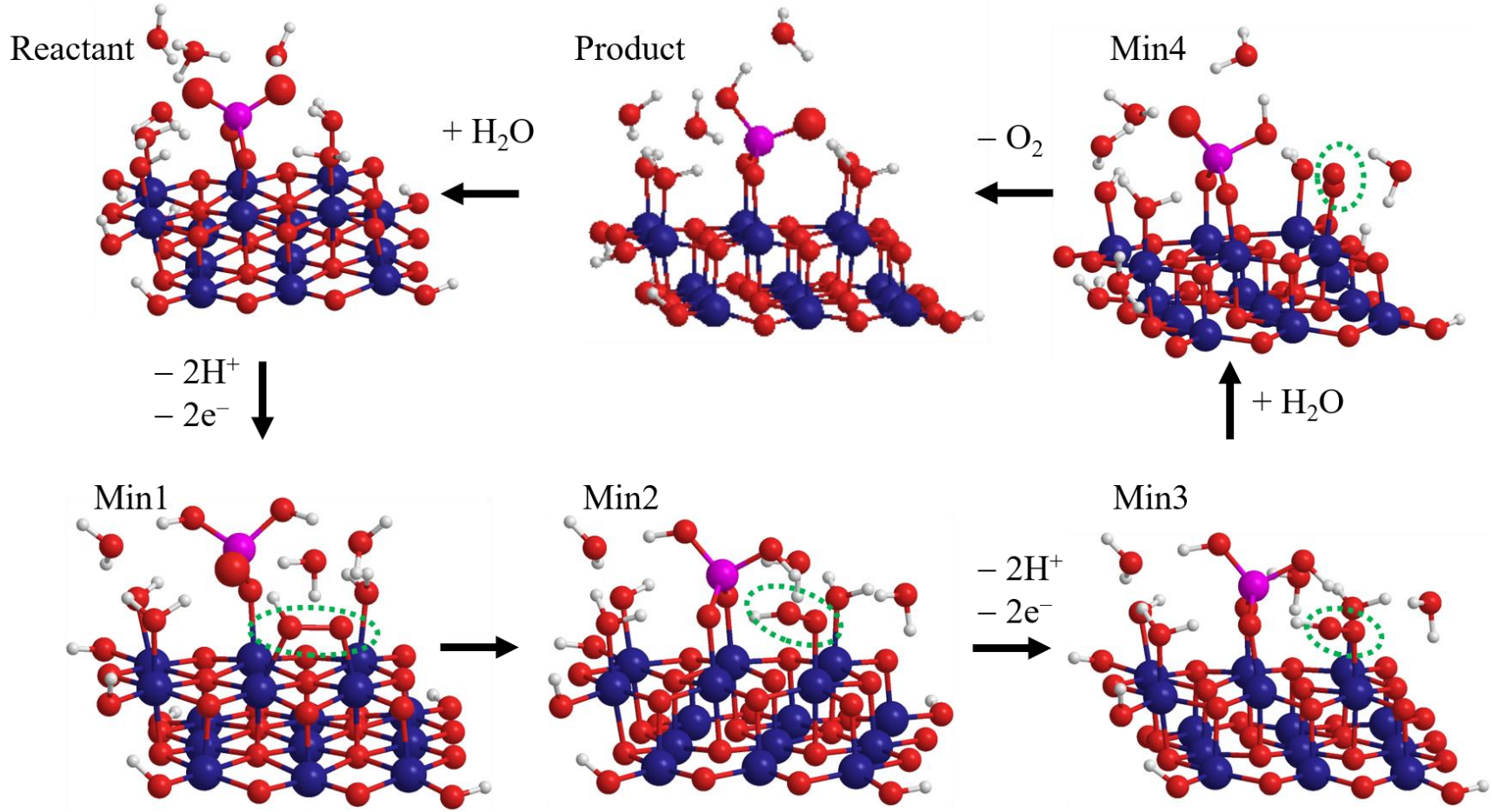

Fig. S4. Water oxidation reaction mechanism of hydrated CoPi surface in the singlet state for the singlet-state cobalt oxide surface. Formed O-O bonds are indicated in green circles.

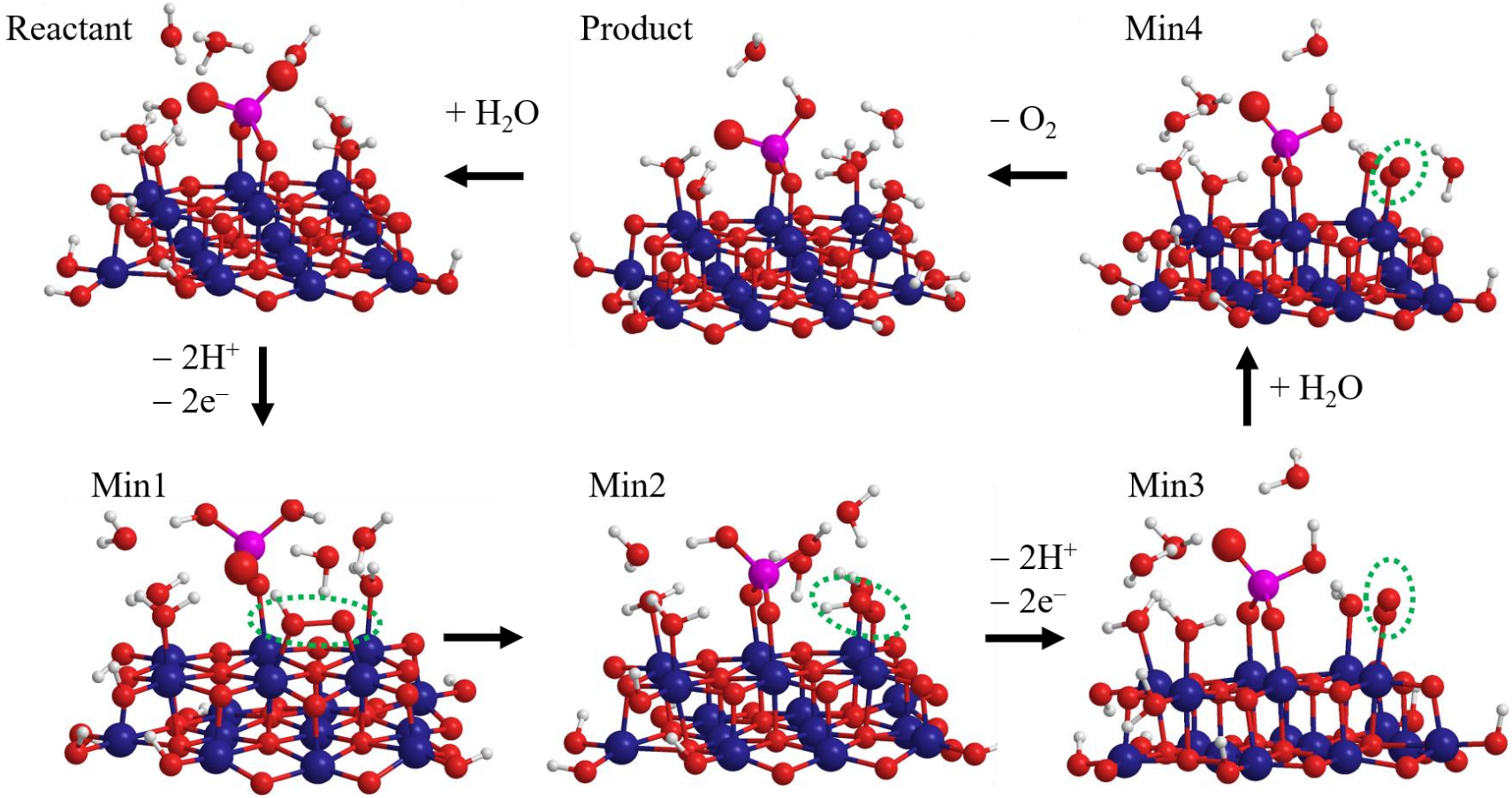

Fig. S5. Water oxidation reaction mechanism of hydrated CoPi surface in the triplet state for the singlet-state cobalt oxide surface. Formed O-O bonds are indicated in green circles.