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Supplementary Information for

Multihole water oxidation catalysis on haematite photoanodes revealed by *operando* spectroelectrochemistry and DFT

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Methods

Preparation of the metal oxide photoanodes

Nanostructured haematite (α-Fe_2O_3) films were deposited by atmospheric pressure chemical vapor deposition (APCVD) following a procedure detailed elsewhere.[1,2] These films exhibit a dendritic structure thickness of ~400 nm and a surface feature size of 5-10 nm with a roughness factor of ~21. This roughness factor was employed to correct the corresponding PIA and TPC data for the rate law analyses. The haematite films studied herein are doped with 1.5% silicon and contains a SiO_2 buffer layer between the FTO glass and the α-Fe_2O_3.

Undoped bismuth vanadate ($BiVO_4$) photoanodes were grown by a metal-organic deposition method with spin-coating as reported previously.[3] This deposition method produces relatively flat and dense films with a roughness factor of ~1.

Dense titania (TiO_2) films were prepared by APCVD at 450 ^oC following a procedure reported previously. This deposition method followed by an annealing process at 500 ^oC produces relatively flat, ~1 μm thick anatase films.[4] Roughness factor ~1.

Tungsten oxide (WO_3) nanosheets photoanodes films were synthesized using a hydrothermal method previously described in the literature.[5]

UV-Vis spectra

Absorption spectra of the α-Fe_2O_3, TiO_2 and $BiVO_4$ films were measured in a UV-Vis spectrometer (Perkin-Elmer, Lambda 25). A Shimadzu UV-vis 2600 spectrophotometer equipped with an integrating sphere was used to measure the spectra for the WO_3 film (see Supplementary Figure 2 for the spectra).

Materials characterization

As described in the previous section all the materials have previously been synthesized and characterized in different publications: α-Fe_2O_3,[1,2] $BiVO_4$,[3] TiO_2[4] and WO_3.[5] As it is indicated in the corresponding publications the morphology of the different films it is varies as follows, $BiVO_4$ is a dense film, α-Fe_2O_3 presents a cauliflower nanostructured form, WO_3 is synthesized in nanosheet form and TiO_2 is a dense, flat electrode. Despite these differences we can qualitatively compare the different behavior towards water oxidation.

The four materials we discuss in this paper present very different photoelectrochemical performances, as is shown in Supplementary Figure 3, respectively. Two clear differences can be easily observed: the onset of the photocatalysis and the steady state current density at high applied potentials. The earliest onset is presented by TiO_2 (0.3 V vs RHE) followed by $BiVO_4$ (0.45 V vs RHE), WO_3 (0.6 V vs RHE) and finally α-Fe_2O_3 (1 V vs RHE). This can be associated with the valence band position (see Figure 1 in the main section) and recombination processes. On the other hand, if we focus on the maximum photocurrent density, the best performing material is α-Fe_2O_3 (3 mA/cm^2) followed by $BiVO_4$ (1.2 mA/cm^2), WO_3 (0.25 mA/cm^2) and TiO_2 (0.022 mA/cm^2). This can be explained by the absorption of the materials (Supplementary Figure 2), being α-Fe_2O_3 the material absorbing more visible light.

Light Induced Spectroelectrochemistry (LI-SEC) setup

Rate laws were performed by means of the simultaneous measurements of the Photo-Induced Absorption (PIA) and the Transient Photocurrent (TPC) responses of the studied photoanodes. These measurements were performed under steady-state illumination and highly oxidative (1.5 V_{RHE}) conditions in a 3-electrode photoelectrochemical (PEC) cell (see Supplementary Figure 3 for the current-potential response of the photoanodes used herein). The PIA signal, proportional to the surface hole density, was acquired by monitoring the change in the absorbance of the photoanode after illumination by two 365 nm Light Emitting Diodes (LedEngin Inc.) delivering a photon flux of 1-70 mW.cm^{-2}, controlled by the passing current. We note that the indication of ~1 sun irradiation conditions in the main text and Supplementary Information refers to the photon flux set to obtain the photocurrent densities typically observed under AM 1.5G irradiation conditions shown in Supplementary Figure 3. The change in optical density was recorded at 650 nm for α-Fe_2O_3,[6] 550nm for $BiVO_4$,[7] 500 nm for TiO_2[4] and 500 nm for WO_3[8] corresponding to the reported absorption maxima of the photogenerated holes in each photoelectrode, which for these photoanodes is ~ 100 nm red shifted compared to their ground state absorption (see Supplementary Figure 1 for the example of α-Fe_2O_3). To convert the optical signal to surface hole density, the molar extinction coefficient for the valence band holes have been reported previously as 640 M^{-1} cm^{-1} for α-Fe_2O_3,[6] 420 M^{-1} cm^{-1} for $BiVO_4$,[7] and 2000 M^{-1} cm^{-1} for TiO_2.[4] We note that tungsten oxide photogenerated holes maximum absorption (see Supplementary Figure 4) and the hole extinction coefficient (see Supplementary Figure 5) are reported herein for the first time measured in diffuse reflectance mode. The TPC signal was measured by a potentiostat (Autolab 101) between the photoanode and a Pt mesh, as working and counter electrodes, respectively while the applied potential between the photanode and a KCl saturated Ag/AgCl reference electrode (E°= 0.197 V vs. NHE) was held at 1.5 V_{RHE} for α-Fe_2O_3, TiO_2, 1.4 V_{RHE} for WO_3 and 1.7 V_{RHE} for $BiVO_4$.

An example of the PIA and TPC for WO_3 data is shown in Supplementary Figure 4 as well as the cited references for α-Fe_2O_3,[6,9] $BiVO_4$[7,10] and TiO_2[4] photoanodes for water and hole scavengers oxidation reactions. The complete optical and electrochemical data set is available in http://zenodo.org with the identifier (10.5281/zenodo.851635).

Turn-over frequencies (TOF) can also be calculated from the kinetic data obtained from the PIA and TPC simultaneous measurements. Figure 1.a in the main text, which shows TOF as a function of surface hole density (h_s^+), was calculated dividing the reaction flux value (J^{ph}) by its corresponding surface hole density (h_s^+) and plotting this TOF with units of s^{-1} versus h_s^+.

Temperature dependence study setup and confirmation of the activation energy

A custom-made heating device was used for the temperature dependence study composed by an aluminum cell insulated with calcium silicate (Duratec 750) of 6 mm width. The temperature was regulated by two resistive heaters (50 W) and a K-type thermocouple linked to a PID controller. The working and counter electrodes were placed in a closed quartz cuvette and the Ag/AgCl reference electrode was placed in a separate container connected by a salt bridge. Therefore, the applied potential was not corrected for temperature.

A quantitative analysis of the kinetic data presented in Figure 2.a in the main section as a function of the temperature can yield to the Arrhenius plot shown in Figure 2.a, inset. This analysis was carried

out calculating the water oxidation rate constant (k_{WO}) for both order reaction regimes from the intercept of the linear fittings of the rate law analysis (see corresponding data in Figure 2.a in the main section):

$$J^{ph} = k_{WO} \cdot (h_s^+)^{\alpha} \qquad \text{Supplementary Equation 1}$$

where J^{ph} is the steady-state photocurrent density, h_s^+ is the surface hole density measured optically and k_{WO} is the observed rate constant for the water oxidation reaction. Alternatively, by replacing the rate constant term for its equivalency according to the Arrhenius equation, Supplementary Equation 1 can be rewritten as:

$$J^{ph} = A \cdot e^{-Ea/k_B \cdot T} \cdot (h_s^+)^{\alpha} \rightarrow Ln(J^{ph}) = \frac{-Ea}{k_B \cdot T} + Ln(A) + Ln(h_s^{+\alpha}) \qquad \text{Supplementary Equation 2}$$

where A is the pre-exponential factor, k_B is the Boltzman constant, T is the temperature and Ea the activation energy. Assuming a constant pre-exponential factor and plotting the natural logarithm of the photocurrent *vs* the inverse of the temperature at a constant surface hole density, the activation energy can also be calculated (see Supplementary Figure 6).

This analysis, for surface hole densities between 0.1 and 1 h^+ nm^{-2}, *i.e.* 1st order of reaction, yields to an activation energy, Ea, of 0.31 ± 0.04 eV, compared to the 0.30 ± 0.04 eV obtained using Supplementary Equation 1 (see Figure 2.a, inset in the main section). For the 3rd order of reaction, *i.e.* above 1 h^+ nm^{-2}, Supplementary Equation 2 yields to an Ea = 0.07 ± 0.01 eV, compared to the 0.06 ± 0.02 eV shown in the main section. This, therefore, confirms the validity of our experimental analysis.

Electrolyte solutions for pH and kinetic isotope effect study

The electrolyte used in the PEC cell varied according to the experiment in the present study as follows: Photoelectrochemical behavior, shown in Supplementary Figure 3, and rate law analysis, shown in Figure 1.b in the main text, were measured in 0.1 M NaOH (pH 13.0) for α-Fe_2O_3, 0.1 M phosphates buffer (pH 6.7) for $BiVO_4$, 1 M NaOH for TiO_2 (pH 13.6) and 0.1 M Na_2SO_4 adjusted with H_2SO_4 to reach the desired pH (pH 3.0) for WO_3. For the temperature dependence study of the 1st and 3rd order mechanisms on haematite the electrolyte used was 0.1 M NaOH (pH 13). Different pH electrolytes (see current-potential response in Supplementary Figure 7 and their respective rate law analyses in Supplementary Figure 8), 0.1 M phosphates buffer, were prepared for the pH dependence study varying the ratio $[H_2PO_4^-]/[HPO_4^{2-}]$ for pH 6.5, 7.2 and 8.4 and from a 0.1 M K_2PO_4 solution conditioning with 1M NaOH for the pH 9.3, 11 and 12.3. Solutions of 0.1 M and 1 M NaOH were prepared for pH 13 and 13.7 respectively. Deuterated electrolytes were prepared with the same ratio or concentrations of >98% deuterated reactants. All the reagents were purchased from Sigma-Aldrich.

The possibility of a Nersntian behavior was evaluated by plotting the onset of catalysis versus the pH (see Supplementary Figure 9). This onset of catalysis was calculated as the applied potential where a change in the 1st derivative of the respective JV curve (Supplementary Figure 7) is most significant.

Computational details

We used the Vienna ab initio simulation package (VASP)[11–14] for periodic boundary calculations. Projector augmented wave (PAW) method[15,16] together with the PBE exchange-correlation functional[17] were employed to describe the electron-ion interactions. A cutoff of 450 eV was chosen for the plane wave basis set in all calculations. The Gaussian smear method was used to speed SCF convergence and the σ value was chosen to be 0.1 eV. All calculations involving Fe atoms were performed with the spin-polarized DFT+*U* method, using the the formalism suggested by Dudarev *et al*,[18] because of the strong d-electron correlation effects for Fe. The parameter was set at U_{eff} = 4.0 eV to reproduce the experimental band gap of α-Fe_2O_3.[19]

A 5 × 5 × 5 Monckhorst-Pack type k-point grid[20] was chosen for the optimization of bulk haematite. The energy convergence criterion was set to be 10^{-4} eV per unit cell and the geometry convergence criterion was set to be 10^{-3} eV per unit cell for energy difference between two consecutive ionic steps.

A slab model of haematite (110) surface were constructed from the optimized bulk haematite structure, which contains four layers of Fe atoms and eight layers for O atoms (Supplementary Figure 10). The lattice constants from the bulk optimization were fixed for all our slab calculations. A previous study[21] shows that haematite (110) surfaces interact strongly with water molecules, forming singly-, doubly-, and triply-coordinated O (OH) sites. Our calculations suggest the chemical adsorption of water molecules on bare haematite (110) surface is strongly exothermic and solvation effects from the bulk solvent is significant (Supplementary Figure 10). Therefore, we constructed a hydroxyl terminated haematite (110) surface model and considered the solvation effect with an implicit solvation model implemented in VASPsol.[22] A value of 80.0 was used to account the dielectric constant of water. A supercell of 8.76 Å × 25.12 Å × 13.83 Å, containing a slab of 174 atoms and a dielectric continuum of ~ 15 Å thickness, was used to model haematite (110) surfaces. The third Fe layer and two layers of O atoms surrounding this Fe layer were frozen at their bulk positions while other atoms were allowed to relaxed during geometry optimization to obtain a fully relaxed hydroxyl terminated haematite 110 surface model. The final haematite (110) slab model contains four layes of Fe atoms, six layers of O atoms, and hydroxide groups on both sides of the slab (Supplementary Figure 11).

The Fe atoms involved in the 1st and 3rd order mechanisms, as well as O atoms coordinated to them are highlighted in Supplementary Figure 10. We note that our pH dependence and the kinetic isotope effect data (Supplementary Figure 8) shows that the water oxidation rate determining step transitions from 1st to a 3rd order in all cases. These data suggest that the protonation state does not affect the reaction mechanism but only the water oxidation rate constant. Therefore, we considered neutral slab model. For all intermediates, we fixed the bottom two layers of Fe atoms and corresponding O atom and surface HO groups while other atoms were allowed to relaxed (Details can be found in the geometries provided in the "Optimized Geometries" section). The energy convergence criterion was set to be 10^{-6} eV per super cell. The force convergence criterion of 0.03 eV $Å^{-1}$ and a 1 × 1 × 1 Monckhorst-Pack type k-point grid was used for all surface structure relaxations unless otherwise noted.

The nudged elastic band (NEB) method[23] was used to get the initial guess for transition states, which were fully optimized with the improved dimer method[24] implemented in VASP. In all surface geometry optimizations, solvation effect was considered with an implicit solvation model implemented in VASPsol. Frequency analysis was performed for all optimized stationary points to verify the nature of those geometries (intermediates or transition states) and to calculate thermal corrections to

enthalpies, entropies, and free energies. Frequencies were calculated by diagonalizing numerical hessian calculated with central difference with a stepsize of 0.015 Bohr. Only two Fe atoms, three OH groups coordinated to those two Fe atoms, and the incoming substrate water molecules when it is present, were included to calculated the numerical hessian matrix. Calculated vibrational frequencies were used to calculate zero-point energies, entropies, thermal contributions to enthalpies and free energies at 298.15 K by standard methods.[25] The calculated ZPEs, entropies, thermal contributions to enthalpies and free energies of intermediates and transition states involved in 1st and 3rd order mechanisms are listed in Supplementary Tables 1-2.

A supercell of 15.0 Å × 15.0 Å × 15.0 Å, the Gaussian smearing method and a σ value of 0.1 eV were used in the calculations of isolated small molecules (H_2, O_2, H_2O, and H_2O_2). For isolated small molecules, we also performed geometry optimization and frequency analysis using PBE with the 6-311+G(2df,p) basis set[26] using Gaussiaon 09 software package.[27] The calculated ZPEs using Gaussian and VASP agree well with each other (Supplementary Table 3). Thus, we used the zero-point energies, entropies, thermal contributions to enthalpies and free energies of isolated small molecules from Gaussian 09 calculations to include the contributions from translational and rotational contributions. They are listed in Supplementary Table 3.

As shown in Supplementary Figure 10, reliable geometries can be obtained from calculations with a 1 × 1 × 1 k-grid and the relative energy evaluated from single point energies calculation with a 3 × 1 × 3 k-grid based on the 1 × 1 × 1 k-grid geometries is essentially the same as that evaluated from much more expensive geometry optimization with a 3 × 1 × 3 k-grid. Therefore, we performed single point enegy calcualtions with a 3 × 1 × 3 Monckhorst-Pack type k-point grid at the geometried optimized with a 1 × 1 × 1 k-grid to obtain refined energetics. Dispsersion interactions were considered using Grimme's D3 correction with the Becke-Johnson damping.[28] Thermal corrections in Supplementary Tables 1-3 were used to obtain free energies and enthalpies. For reaction steps involving the H^+ and e^-, the computational hydrogen electrode (CHE) technique developed by Nørskov *et al.*[29] was used to calculated the free energy changes and the corresponding oxidation potentials were therefore relative to reversible hydrogen electrode (RHE). The calculated free energy profiles for the 1st and 3rd mechanisms are shown in Supplementary Figure 13-15. We obtained the free energies profiles of 1st and 3rd order mechanisms shown in Figure 3.a, 3.b, and Supplementary Figure 12, to make better comparison to experiments, assuming haematite provides a photovoltage of 0.80 V.[30] We also changed H to D to perform frequency analysis to obtain thermal corrections to free energies for D-substituted species (Supplementary Table 1-3) and applied transition state theory to estimatedthe H/D kinetic isotope effect (KIE). Our estimation of H/D KIEs of the 1st and 3rd order mechanisms are 1.03 and 2.50, respectively, consistent with experimental observed ones.

1st order discussion

Under low illumination, the photogenerated holes were found to react with 1st order kinetics. This mechanism, which operates only at low surface hole densities, must involve only a single Fe^{IV}=O species in the rate determining step (rds) of the reaction. We found a low activation energy pathway for this reaction via formation of hydrogen peroxide Fe^{II}-HOOH species (see Figure 3.a in the main text), which could be subsequently replaced by a water molecule to release hydrogen peroxide or oxidized to release oxygen. Our calculations indicate that Fe^{IV}=O abstracts a hydrogen atom from the incoming substrate water molecule with a activation free energy of 0.41 eV to form a surface bound hydroxyl radical (intermediate **III**) which lies 0.38 eV higher than separated reactants, and the subsequent O-O bond formation has an activation free energy of 0.16 eV. Thus, the overall activation

free energy of the O-O bond formation is 0.54 eV. The activation enthalpy (0.26 eV) is found to be consistent with the activation energy (0.3 eV) experimentally obtained in the Arrhenius plot shown in the inset in Figure 2.a in the main text.

We noted that if the hole diffusion rate is faster than than the substitution rate of H_2O_2 by H_2O, the generated H_2O_2 bound intermediate (**IV**) can be further oxidized before it could be released to the aqueous solution. We explored both possibilities and the calculated energetics are presented in Figure 3.a. and Supplementary Figure 12. The further oxidization of the bound H_2O_2 to produce O_2 is thermodynamically feasible. Therefore, if the hole diffusion is fast enough, the in situ generated H_2O_2 will be oxidized to O_2 and no free H_2O_2 could be detected in solution. However, in both mechanistic pictures, the H_2O_2 bound intermediate (**IV**) is produced by the reaction of H_2O with Fe(IV)=O with a first order dependence on the hole density, corresponding to the experimental observed first order kinetics.

Comment on alternative haematite rate law analysis by Zhao et al.[31]

Zhao and co-workers,[31] have reported a rate law and a mechanistic study of water oxidation on a nanorod haematite photoanode by attenuated total reflectance infrared spectroscopy (ATR-IR) and electrochemical impedance spectroscopy (EIS) under photoelectrochemical water oxidation conditions. For the rate law analysis in their study, the authors use an alternative, impedance based, assay of surface hole density. They propose a water oxidation reaction that transitions from a 1st order at low pH values to an order of reaction of 2.5 with respect to surface hole densities at higher pH values. We note however that the interpretation of impedance data is sensitive to details of the kinetic model, as we have discussed previously.[32] Moreover, as this approach is based only upon J/V data, and therefore requires the observation of electron flow to the external circuit for n-type photoanodes such as haematite, it is challenging to use this approach to determine surface hole densities. This contrasts to our optical assay, which is a more direct measurement of the surface hole density, independent of the kinetic model. On the other hand, the assignment of an FT-IR signal at ~1100 cm^{-1} to the stretch vibration of a superoxide species (Fe^{III}-O-H···$O^{\bullet}$-O-Fe^{III}) is in agreement with the water oxidation reaction proposed herein (Supplementary Figure 16).

1st and 3rd order rate constant units

The rate constant units for the 1st order reaction are derived as follows from the rate law (shown in equation 1 in the main text):

$$J^{ph} = k_{WO} \cdot (h_s^+)^1 \rightarrow k_{WO} = \frac{J^{ph}}{h_s^+} \qquad \text{Supplementary Equation 3}$$

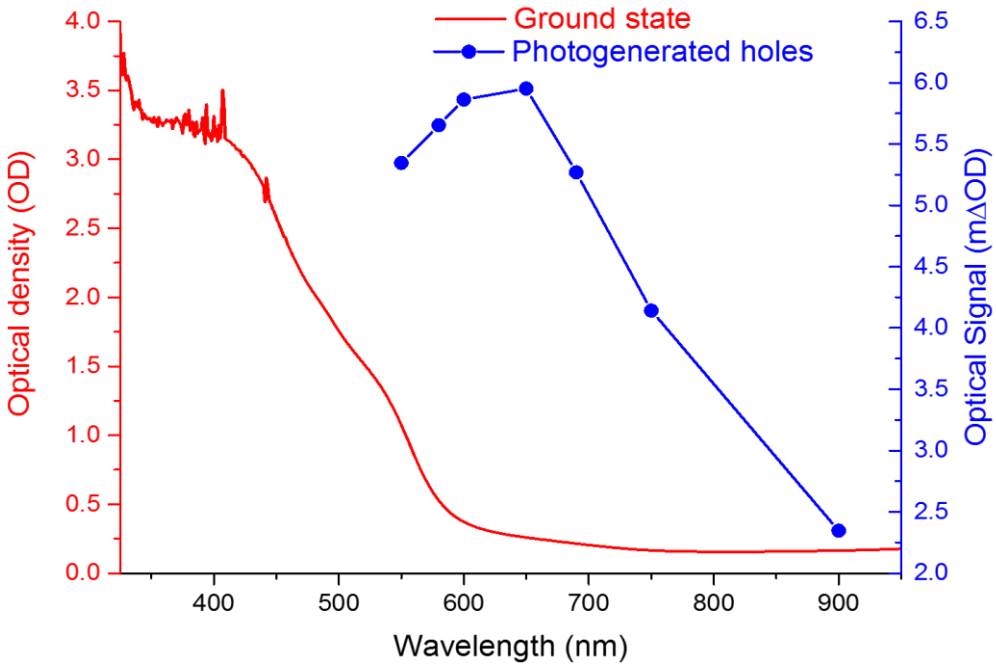
where the photocurrent, J^{ph}, has units of *electrons* s^{-1} nm^{-2} and the surface hole density, h_s^+, has units of *holes* nm^{-2}, therefore, assuming that one extracted electron corresponds to one hole transferred, the rate constant units are:

$$k_{WO} = \frac{electrons \cdot s^{-1} \cdot nm^{-2}}{holes \cdot nm^{-2}} = \boldsymbol{s^{-1}} \qquad \text{Supplementary Equation 4}$$

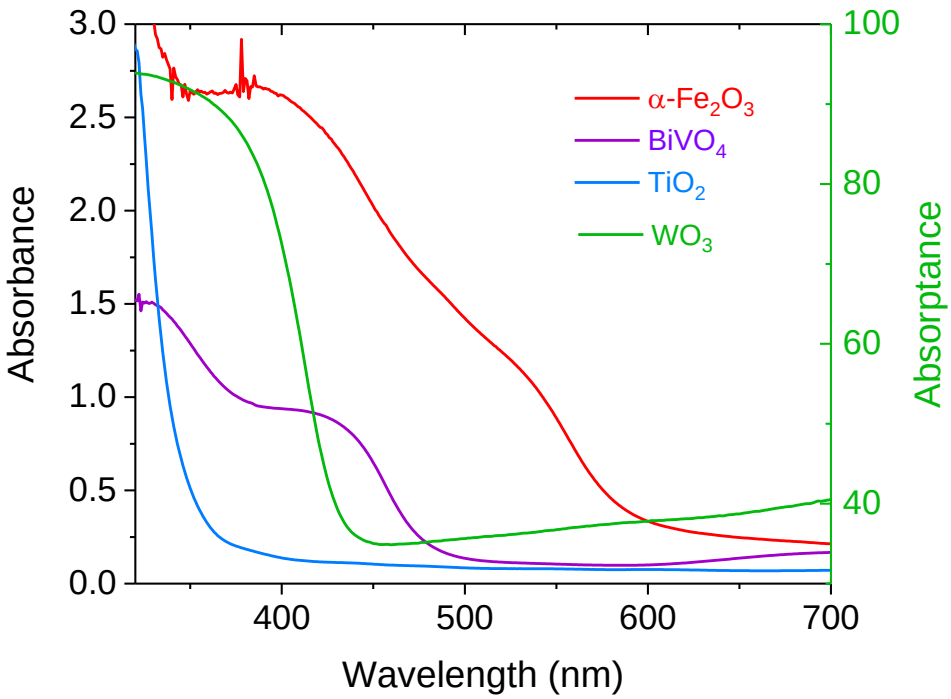
The rate constant units for the 3rd order reaction are derived as follows:

$$k_{WO} = \frac{J^{ph}}{(h_s^+)^3} \rightarrow k_{WO} = \frac{electrons \cdot s^{-1} \cdot nm^{-2}}{(holes \cdot nm^{-2})^3} = \boldsymbol{holes^{-2} \cdot s^{-1} \cdot nm^4} \qquad \text{Supplementary Equation 5}$$

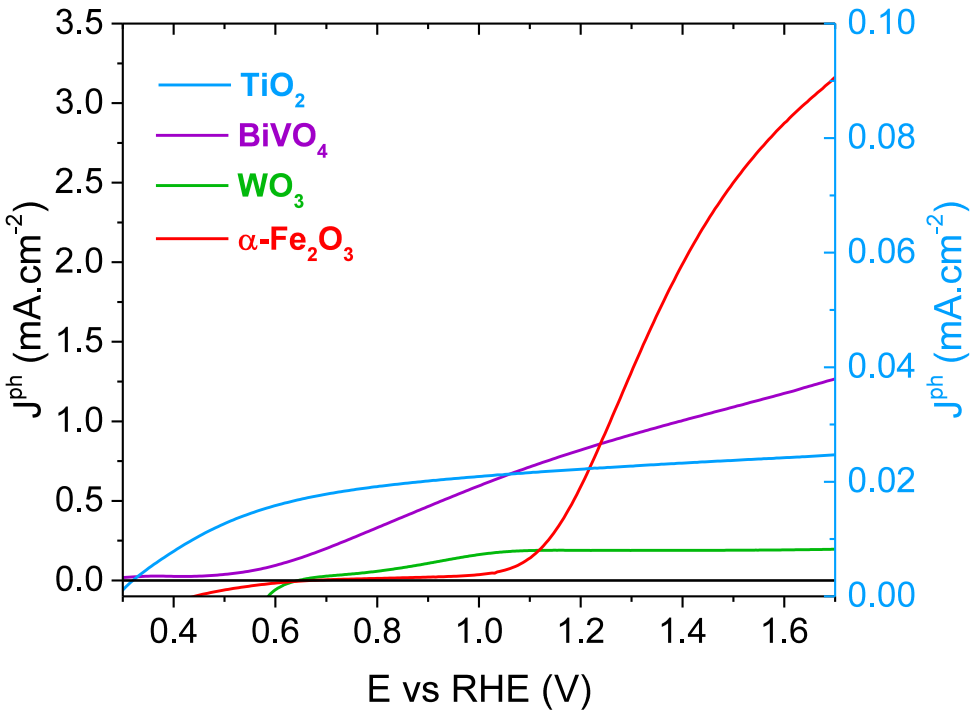
Supplementary Figures



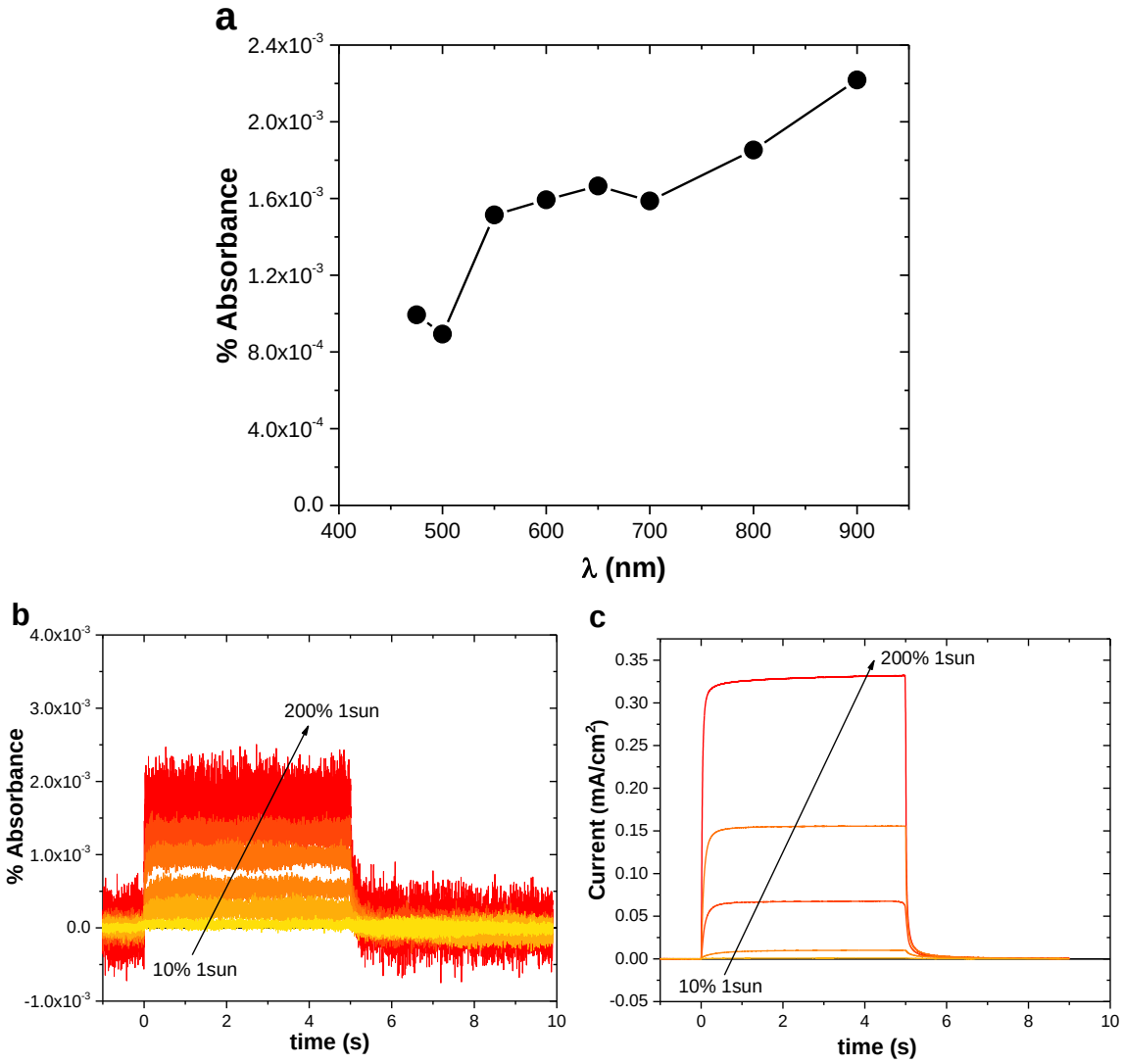
Supplementary Figure 1. Ground state (red) and surface valence band holes (blue) absorption spectra for α-Fe_2O_3. Surface valence band holes spectra was measured in 0.1M NaOH under 1.5 V_{RHE} applied potential.



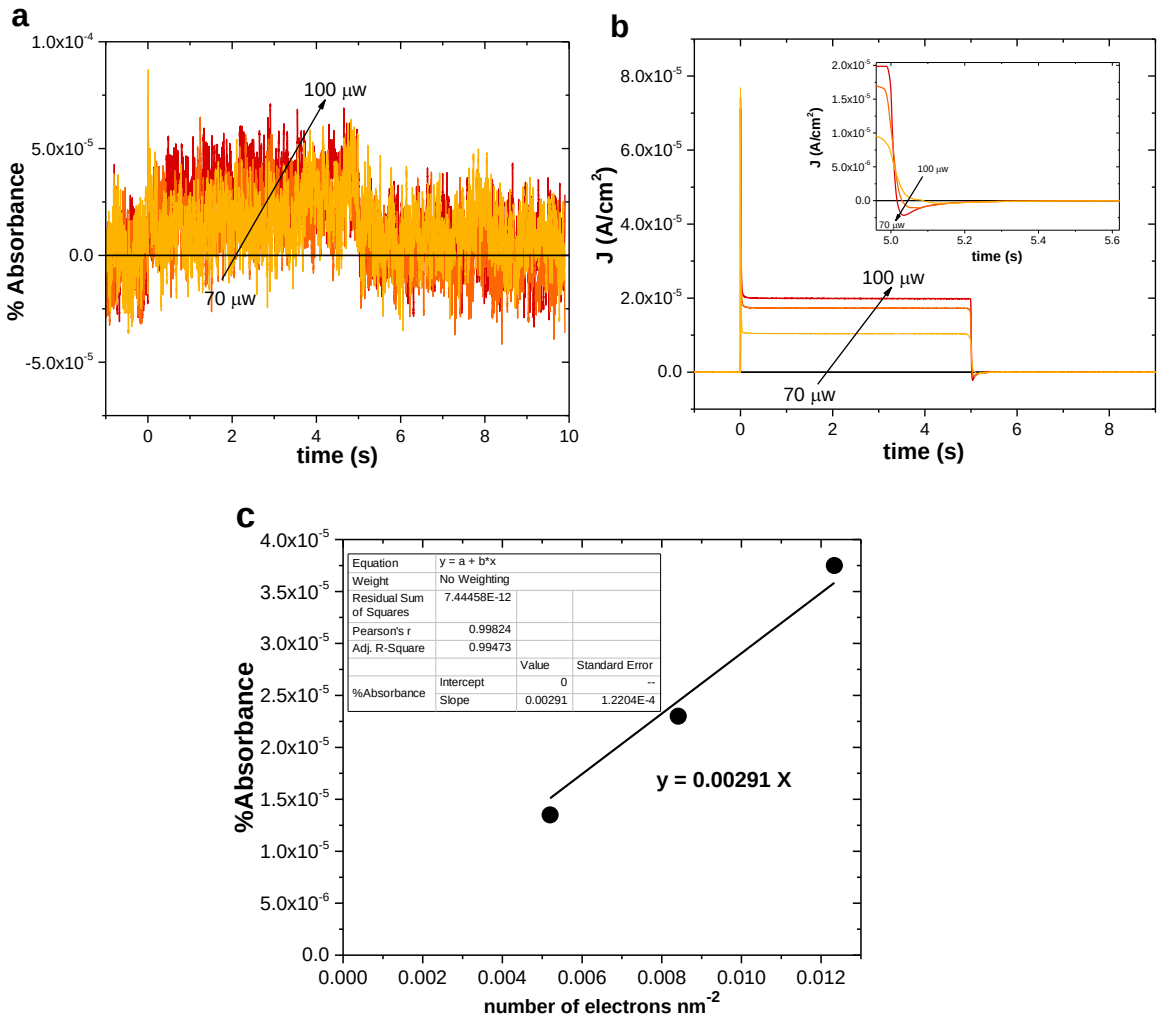
Supplementary Figure 2. UV-Vis spectra of α-Fe_2O_3 (red), $BiVO_4$ (purple), TiO_2 (blue) acquired in transmittance mode and WO_3 (green) acquired in diffuse reflectance mode.



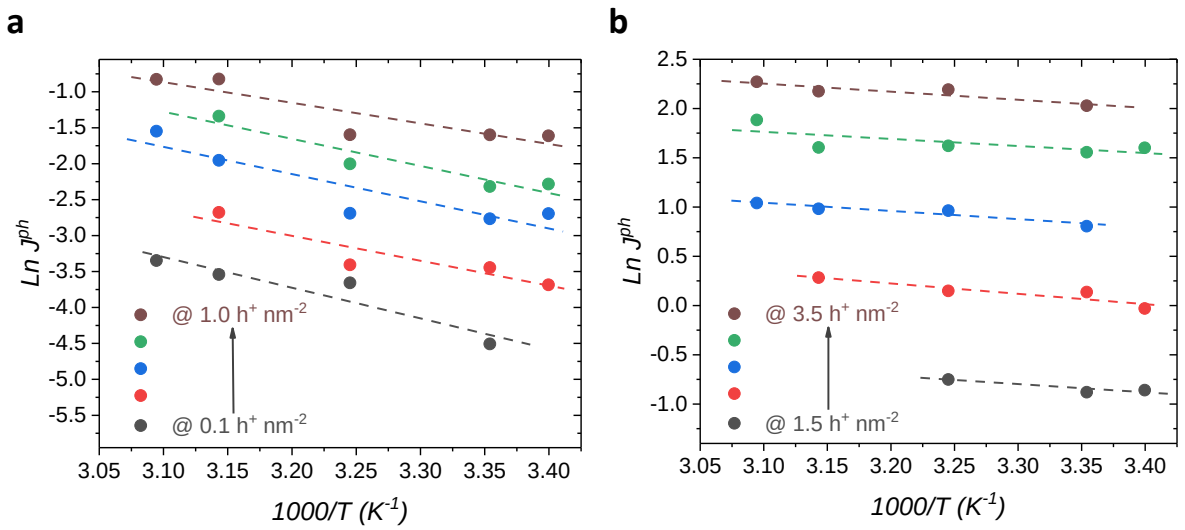
Supplementary Figure 3. Linear Sweep Voltammetry (LSV) under approximately one sun irradiation (Xe-lamp) of α-Fe_2O_3 (red) in 0.1 M NaOH pH 13, $BiVO_4$ (purple) in phosphates buffer pH 6.7, TiO_2 (blue) in 0.1 M NaOH pH 13 and WO_3 (green) 0.1 M Na_2SO_4 adjusted with H_2SO_4 to pH 3.



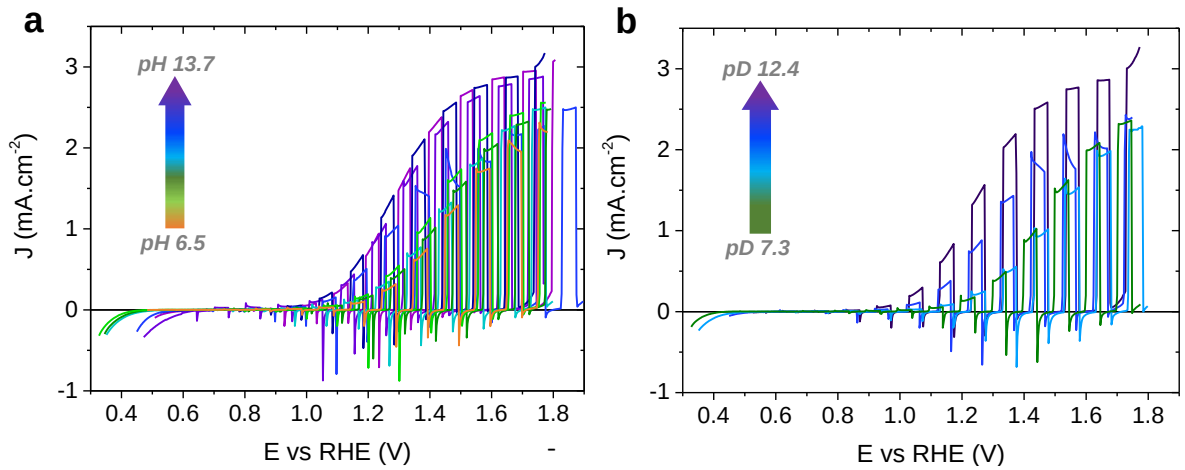
Supplementary Figure 4. PhotoInduced Absorbance and transient photocurrent for WO_3. Data monitored at pH 3 applying 1.4 VRHE. a) PIA spectra under 1 sun irradiation. b) Optical data acquired at 500 nm using different 365 nm LED light intensities. c) Transient photocurrent measured simultaneously as the optical data plotted in (b).



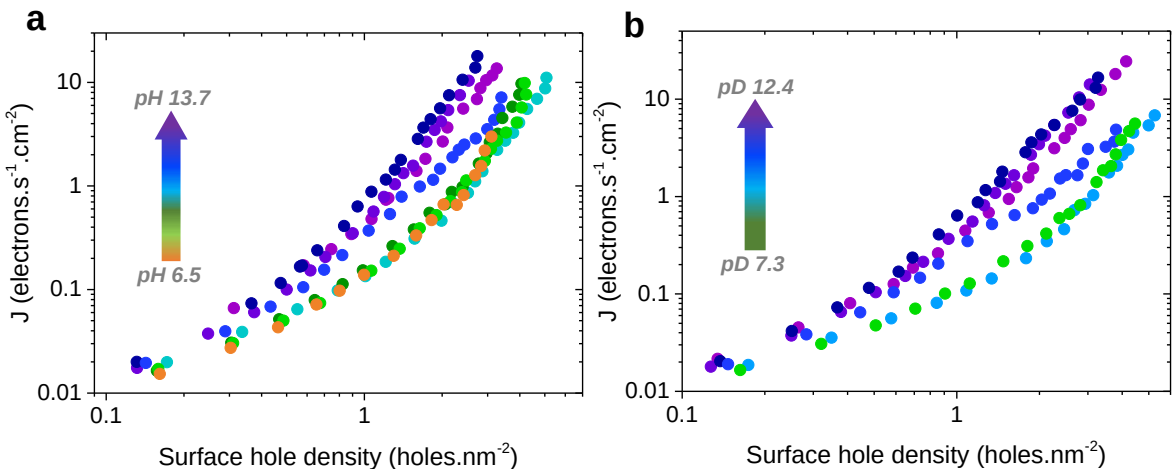
Supplementary Figure 5. Estimation of extinction coefficient of WO_3 holes at 500 nm following the procedure reported in the literature.[6] This was carried out applying 0.78 V_{RHE} and very low light intensities (70 to 100 µW 365 nm LED irradiation) to favor the charge recombination, in a pH 3 electrolyte. The measurements were performed by 5 s illumination and 5 s dark periods a) % absorbance change by time; b) transient photocurrent changes during this time; c) relation between the final %absorbance in a) and the recombined charges when the light was turned off b) inset.



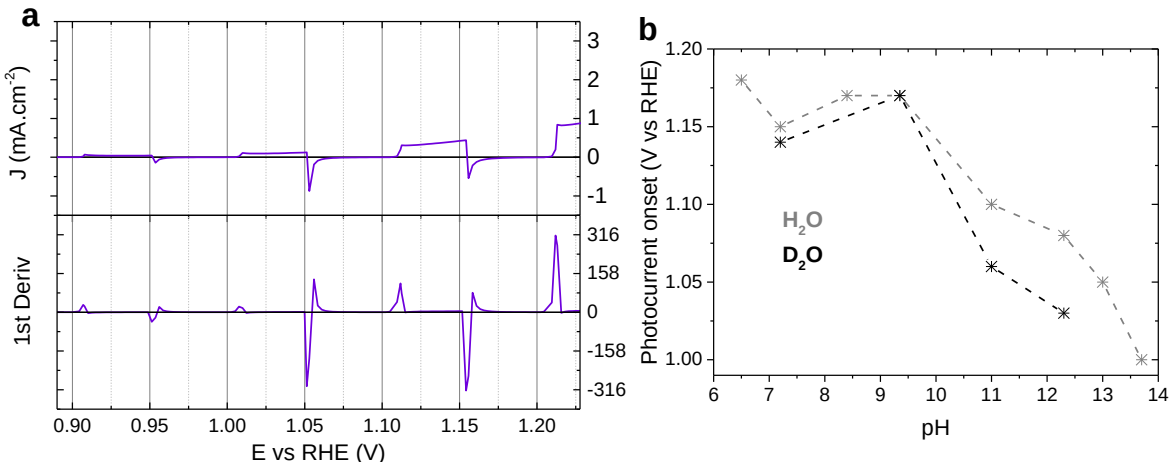
Supplementary Figure 6. Arrhenius plot derived from Supplementary Equation 2 where the natural logarithm of the photocurrent J^{ph} is plotted *vs* the inverse of the temperature for a) the 1st order (from 0.1 to 1 h^+ nm^{-2}) and b) the 3rd order (from 1.5 to 3.5 h^+ nm^{-2}) of the water oxidation reaction on α-Fe_2O_3 photoanodes, respectively. The range of temperatures were between 21 and 50 °C.



Supplementary Figure 7. Chopped LSV of α-Fe_2O_3 in electrolytes of a range of pH between 6.5 and 13.7 as described in the methods section for a) non-deutarated and b) deuterated electrolytes respectively. For the H_2O and D_2O electrolytes the plateau photocurrents reached at highly oxidative potentials are higher when the point of zero charge (pzc 9-10)[33] of the haematite has been surpassed.

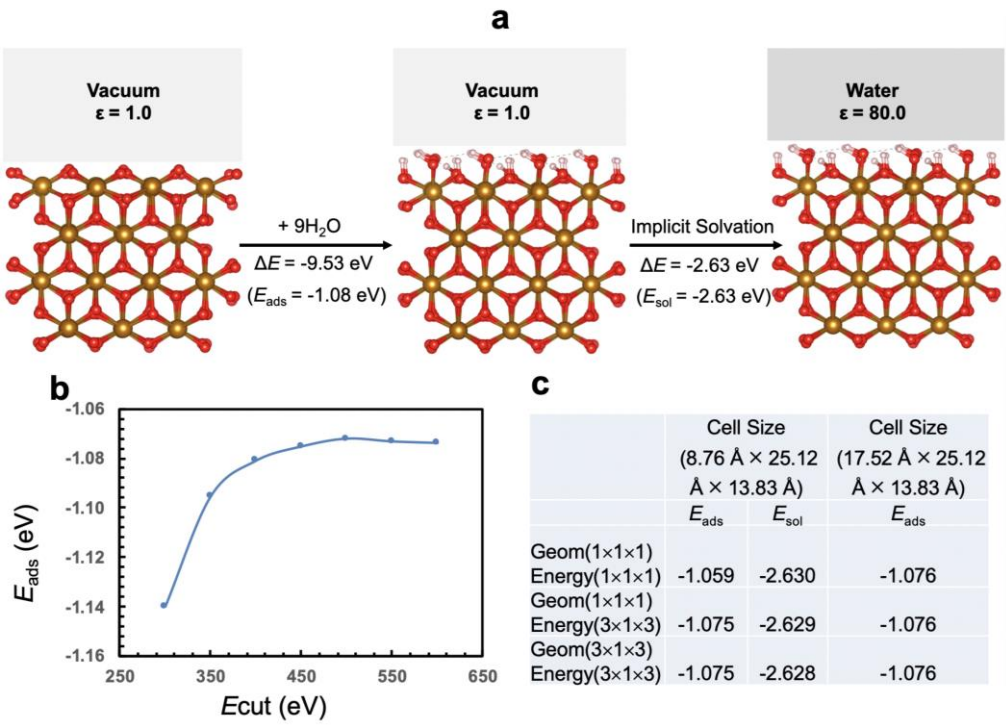


Supplementary Figure 8. Rate law analysis for the oxidation of water for α-Fe_2O_3 at different pH conditions for a) non-deuterated and b) deuterated electrolytes respectively.



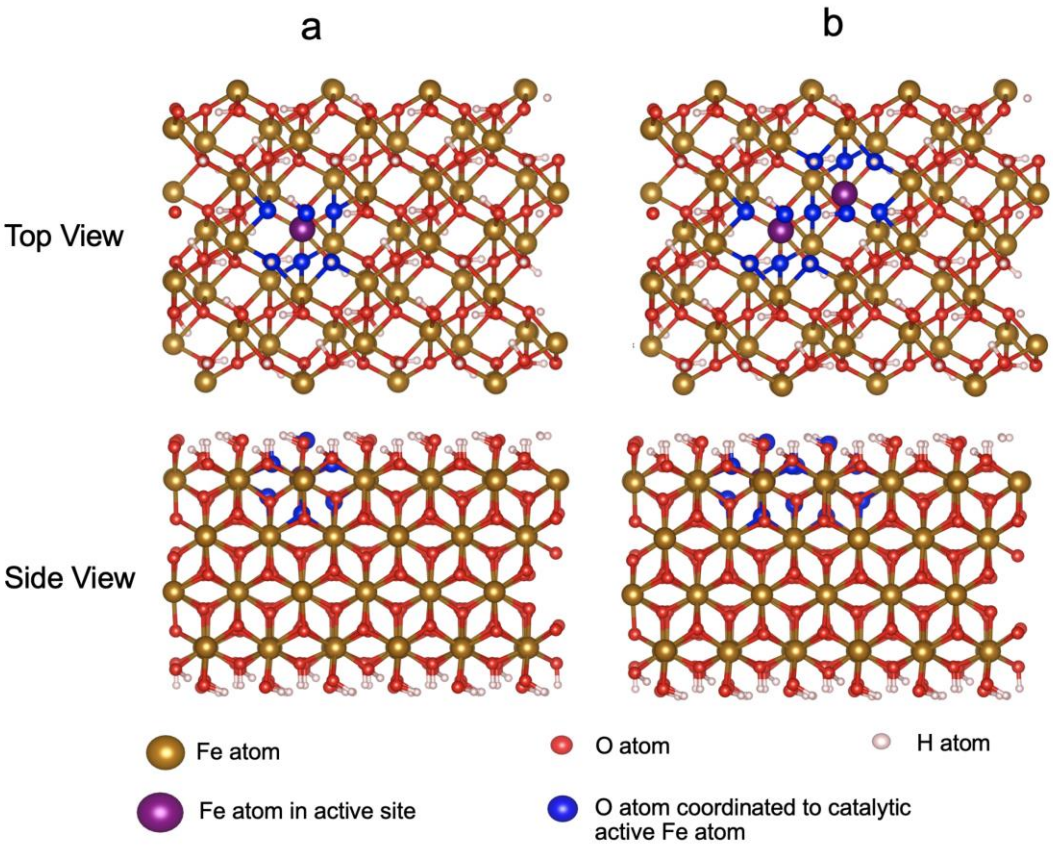
Supplementary Figure 9. Onset of photocatalysis of α-Fe_2O_3 plotted as a function of the pH for the JV curves shown in Supplementary Figure 7. The photocurrent onset is taken as the applied potential where a change in the 1st derivative of the JV curve is most significant as shown in a) zoom in of JV curve (top) and 1st derivative of the JV curve for α-Fe_2O_3 in 0.1 M NaOH pH 13.0 (bottom) and b) photocurrent onset of haematite as a function of the pH for H_2O and D_2O electrolytes.

Computational Supporting data

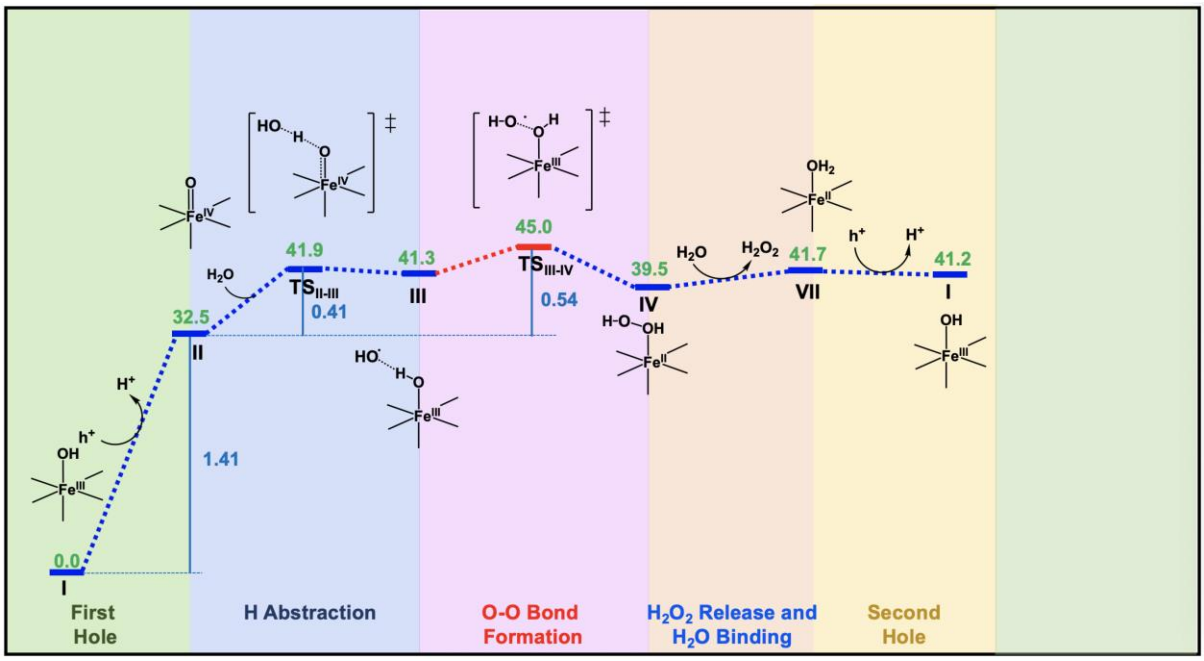


	Cell Size (8.76 Å × 25.12 Å × 13.83 Å)		Cell Size (17.52 Å × 25.12 Å × 13.83 Å)
	E_{ads}	E_{sol}	E_{ads}
Geom(1×1×1) Energy(1×1×1)	-1.059	-2.630	-1.076
Geom(1×1×1) Energy(3×1×3)	-1.075	-2.629	-1.076
Geom(3×1×3) Energy(3×1×3)	-1.075	-2.628	-1.076

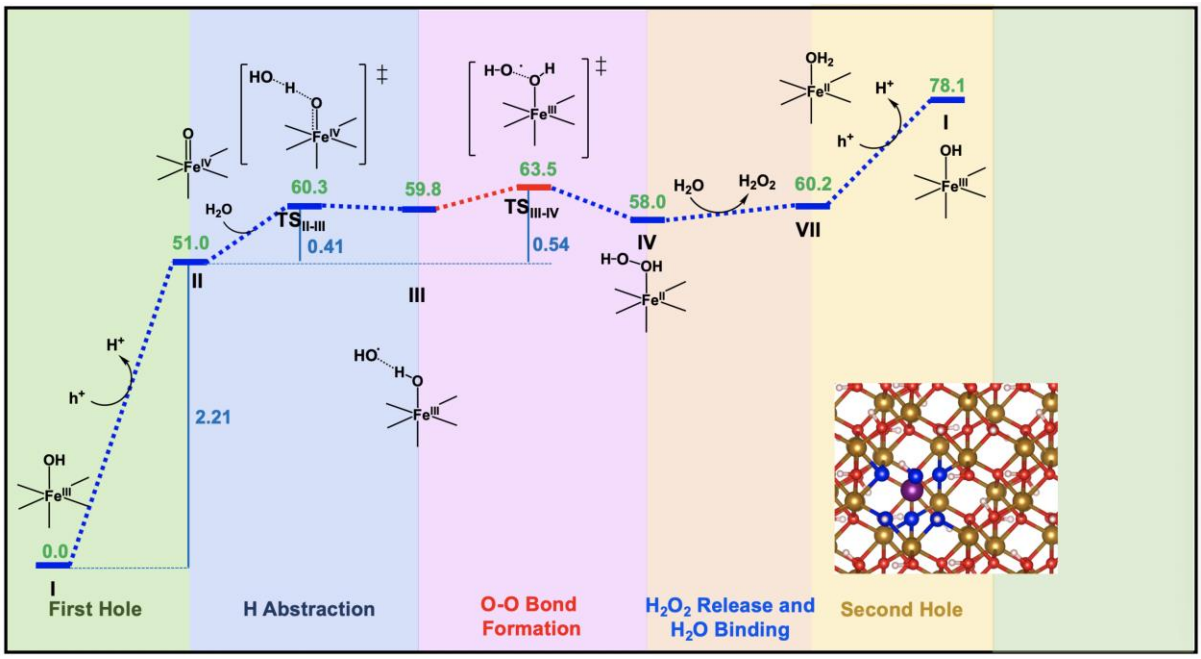
Supplementary Figure 10. Test calculations of water adsorption, bulk solvation, and numerical convergence. a) Calcuated energy changes of adding 9 water molecules to the supercell of haematite (110) surface and solvating the surface by water solvent with an implicit solvation model; b) the calculated water adsorption energy (E_{ads}) with respect to the cutoff energy E_{cut} using 3 × 1 × 3 k-grid and a cell size of 8.76 Å × 25.12 Å × 13.83 Å; (**c**) calculated water adsorption energy (E_{ads}) and solvation energy (E_{sol}) using different k-grid and cell sizes with a cut off energy of 450 eV.



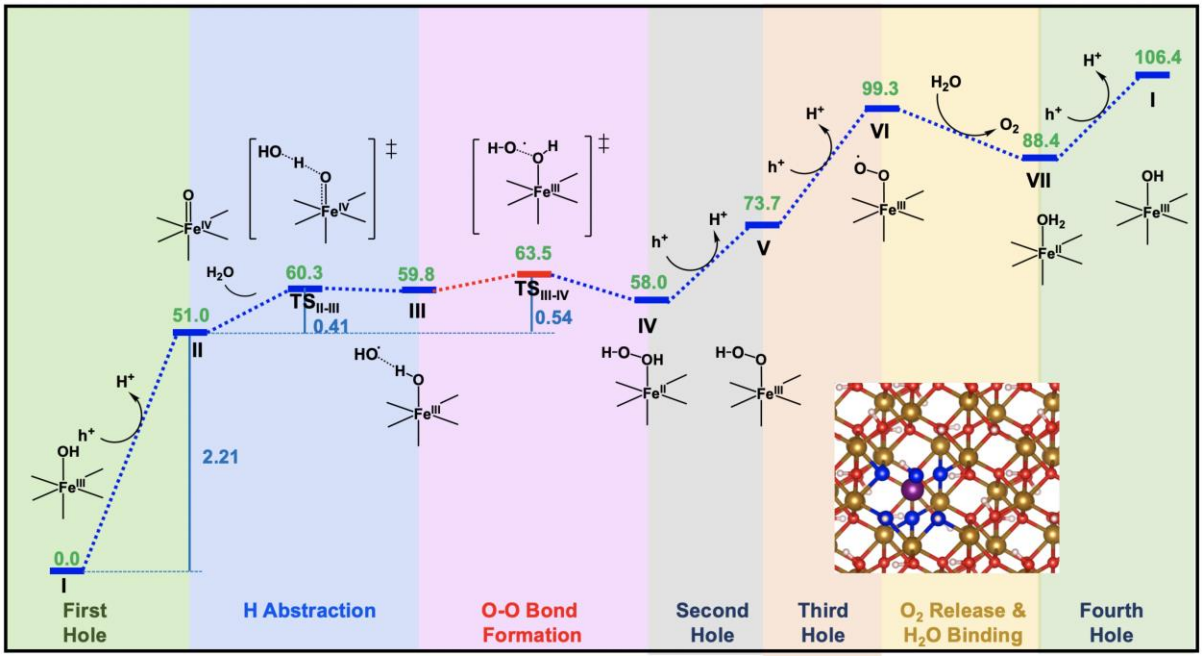
Supplementary Figure 11. Structure of the hydroxyl terminated haematite (110) surface. a) Fe atom and its ligands involved in the 1st order mechanism; b) Fe atoms and their ligands involved in the 3rd order mechanism.



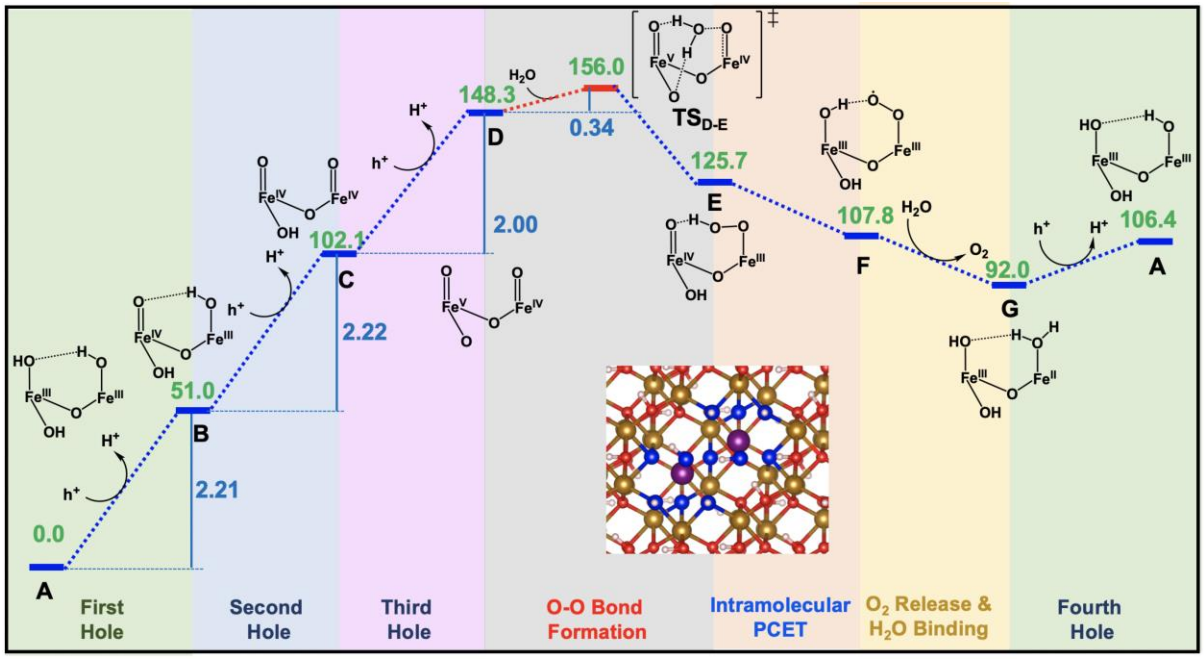
Supplementary Figure 12. Calculated free energy profile of the 1st order mechanism producing the H_2O_2 product (Relative free energies are given in green in the unit of kcal/mol and free energy changes are given in blue in the unit of eV; rate-determining steps are shown in red; a photovoltage of 0.80 V is used for all oxidation steps).



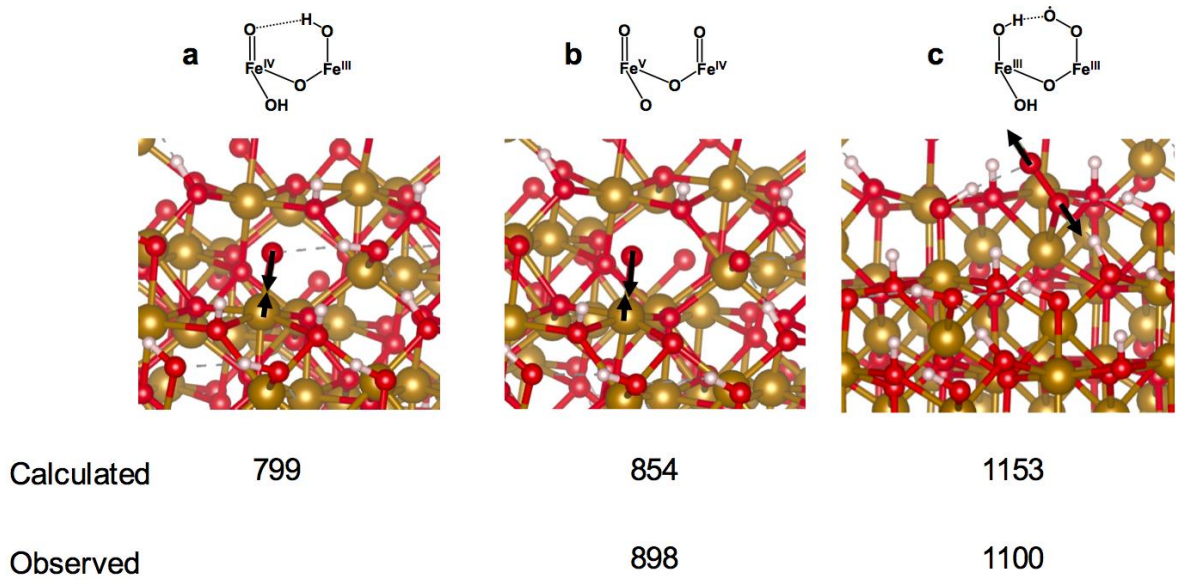
Supplementary Figure 13. Calculated free energy profile of the 1st order mechanism producing the H_2O_2 product (Relative free energies are given in green in the unit of kcal/mol and free energy changes are given in blue in the unit of eV; rate-determining steps are shown in red). The inset shows the Fe monomer embedded in the haematite surface.



Supplementary Figure 14. Calculated free energy profile of the 1st order mechanism producing the O_2 product (Relative free energies are given in green in the unit of kcal/mol and free energy changes are given in blue in the unit of eV; rate-determining steps are shown in red). The inset shows the Fe monomer embedded in the haematite surface.



Supplementary Figure 15. Calculated free energy profile of the 3rd order mechanism (Relative free energies are given in green in the unit of kcal/mol and free energy changes are given in blue in the unit of eV; rate-determining steps are shown in red). The inset shows the Fe dimer embedded in the haematite surface.



Supplementary Figure 16. Calculated vibrational frequencies (in cm^{-1}) and normal modes of (a) Fe^{IV}=O, (b) Fe^{V}=O, and (c) O-O stretching in Intermediates **B**, **D**, and **F**. Experimental observed vibrational frequencies of high-valent Fe-oxo stretching at 898 cm^{-1} and O-O stretching of superoxo at 1100 cm^{-1} are taken from refs[31,34]

Supplementary Table 1. Zero-point energy (ZPE) corrections (calculated with both VASP and Gaussian), entropy (*TS*), enthalpic temperature correction (*H*(*T*) – *E*), and the total free energy correction (*G*(T) - *E*) of surface species in the 1st order mechanism at *T* = 298.15 K. All values are given in eV.

	ZPE	*TS*	*H(T) - E*	*G(T) - E*
I	1.205	0.346	1.436	1.091
II	0.932	0.306	1.141	0.836
TSII-III	1.466	0.441	1.740	1.299
III	1.535	0.468	1.823	1.355
TSIII-IV	1.541	0.425	1.811	1.385
IV	1.597	0.426	1.870	1.443
V	1.307	0.389	1.560	1.171
VI	0.972	0.410	1.230	0.820
VII	1.513	0.388	1.767	1.379
II (D2O)	0.756	0.326	0.978	0.652
TSIII-IV (D2O)	1.190	0.461	1.481	1.020

Supplementary Table 2. Zero-point energy (ZPE) corrections (calculated with both VASP and Gaussian), entropy (*TS*), enthalpic temperature correction (*H*(*T*) – *E*), and the total free energy correction (*G*(T) - *E*) of surface species in the 1st order mechanism at *T* = 298.15 K. All values are given in eV.

	ZPE	*TS*	*H*(*T*) - *E*	G(*T*) - *E*
A	1.205	0.346	1.436	1.091
B	0.932	0.306	1.141	0.836
C	0.647	0.281	0.842	0.562
D	0.337	0.265	0.522	0.257
TS_{D-E}	0.885	0.358	1.120	0.762
E	1.021	0.356	1.252	0.895
F	0.974	0.423	1.237	0.814
G	1.491	0.370	1.734	1.364
D (D2O)	0.337	0.265	0.522	0.257
TS_{D-E} (D2O)	0.731	0.372	0.975	0.603

Supplementary Table 3. Zero-point energy (ZPE) corrections (calculated with both VASP and Gaussian), entropy (*TS*), enthalpic temperature correction (*H*(*T*) – *E*), and the total free energy correction (*G*(T) - *E*) of small molecules at T = 298.15 K. All values are given in eV.

	ZPE(VASP)	ZPE(Gaussian)	*TS*	*H*(*T*) - *E*	*G*(*T*) - *E*
H_2(g)	0.268	0.268	0.403	0.358	-0.045
O_2(g)	0.097	0.097	0.634	0.187	-0.447
H_2O_2(g)	0.699	0.699	0.703	0.812	0.109
H_2O(g)	0.568	0.565	0.584	0.668	0.084
D_2O (g)	0.412	0.411	0.515	0.613	-0.099
H_2O_2(aq)	0.699	0.699	0.703	0.812	0.191 [a]
H_2O(l)	0.568	0.565	0.584	0.668	0.270 [b]
D_2O (l)	0.412	0.411	0.515	0.613	0.087 [b]

[a] Free energy correction included the concentration correction from the standard state of H_2O_2 (g) (1 atm, 0.041 M) to the standard state of H_2O_2(aq) (1M).
[b] Free energy correction included the concentration correction from the standard state of H_2O(g) (1 atm, 0.041 M) to the standard state of H_2O(l) (pure liquid water, 55.6 M).

Optimized Geometries:

The optimized geometries are shown in VASP format.

Small molecules:

H_2 molecule
```
   1.00000000000000
    15.0000000000000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.0000000000000000    0.0000000000000000
     0.0000000000000000    0.0000000000000000   15.0000000000000000
   H
     2
Direct
  0.5020912676691864  0.4326519086666636  0.4666666666666686
  0.5521433029974858  0.4326519086666636  0.4666666666666686
```

O_2 molecule
```
   1.00000000000000
    15.0000000000000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.0000000000000000    0.0000000000000000
     0.0000000000000000    0.0000000000000000   15.0000000000000000
   O
     2
Direct
  0.4943350786540748  0.4326519086666636  0.4666666666666686
  0.5765661586792632  0.4326519086666636  0.4666666666666686
```

H_2O molecule (optimized in gas phase)
```
   1.00000000000000
    15.0000000000000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.0000000000000000    0.0000000000000000
     0.0000000000000000    0.0000000000000000   15.0000000000000000
   O    H
     1     2
Direct
  0.4940630064673588  0.4311606392653188  0.4666666666666686
  0.5588203813383091  0.4339774079957167  0.4666666666666686
  0.4751048288610030  0.4931467340722889  0.4666666666666686
```

H_2O molecule (Optimized in dielectric medium)
```
   1.00000000000000
    15.0000000000000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.0000000000000000    0.0000000000000000
     0.0000000000000000    0.0000000000000000   15.0000000000000000
   O    H
     1     2
Direct
  0.4940630064673588  0.4311606392653188  0.4666666666666686
  0.5588203813383091  0.4339774079957167  0.4666666666666686
  0.4751048288610030  0.4931467340722889  0.4666666666666686
```

H_2O_2 molecule (Optimized in dielectric medium)
```
   1.00000000000000
    15.0000000000000000    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.0000000000000000    0.0000000000000000
```

```
    0.0000000000000000    0.0000000000000000   15.0000000000000000
   O    H
    2    2
Direct
  0.4676629178763534  0.4710923694121973  0.4696310725157886
  0.5656704154569852  0.4696310725157886  0.4710923694121973
  0.4576142660241374  0.5345354896441492  0.4580744017611948
  0.5757190673092012  0.4580744017611948  0.5345354896441492
```

Bare haematite (110) surface (Optimized in gas phase):

```
AFM Fe2O3 110 A termination
   1.00000000000000
    8.7609063200000001    0.0000000000000000    0.0000000000000000
    0.0000000000000000   25.1162232400000001    0.0000000000000000
    0.0000000000000000    0.0000000000000000   13.8345004800000009
   Fe   O
    48   72
Selective dynamics
Direct
  0.8333333337138100  0.1006941125595731  0.0208726741104570   F   F   F
  0.8333333337138100  0.1006941125595731  0.3124606592228787   F   F   F
  0.8333333337138100  0.1006941125595731  0.5208726741104570   F   F   F
  0.8333333337138100  0.1006941125595731  0.8124606592228787   F   F   F
  0.5000000000000000  0.1006941125595731  0.1457939925562073   F   F   F
  0.5000000000000000  0.1006941125595731  0.3542060074437927   F   F   F
  0.5000000000000000  0.1006941125595731  0.6457939925562073   F   F   F
  0.5000000000000000  0.1006941125595731  0.8542060074437927   F   F   F
  0.1666666662861900  0.1006941125595731  0.1875393407771213   F   F   F
  0.1666666662861900  0.1006941125595731  0.4791273258895430   F   F   F
  0.1666666662861900  0.1006941125595731  0.6875393407771213   F   F   F
  0.1666666662861900  0.1006941125595731  0.9791273258895430   F   F   F
  0.6666666662861900  0.2013882251191532  0.1875393407771213   F   F   F
  0.6666666662861900  0.2013882251191532  0.4791273258895430   F   F   F
  0.6666666662861900  0.2013882251191532  0.6875393407771213   F   F   F
  0.6666666662861900  0.2013882251191532  0.9791273258895430   F   F   F
  0.3333333337138100  0.2013882251191532  0.0208726741104570   F   F   F
  0.3333333337138100  0.2013882251191532  0.3124606592228787   F   F   F
  0.3333333337138100  0.2013882251191532  0.5208726741104570   F   F   F
  0.3333333337138100  0.2013882251191532  0.8124606592228787   F   F   F
  0.0000000000000000  0.2013882251191532  0.1457939925562073   F   F   F
  0.0000000000000000  0.2013882251191532  0.3542060074437927   F   F   F
  0.0000000000000000  0.2013882251191532  0.6457939925562073   F   F   F
  0.0000000000000000  0.2013882251191532  0.8542060074437927   F   F   F
  0.8309558287699730  0.3046490521870098  0.0223729608521239   T   T   T
  0.8294165084910858  0.3012053567841591  0.3138857482197892   T   T   T
  0.8372501589365342  0.3012053567841591  0.5194475851135465   T   T   T
  0.8357108386576471  0.3046490521870098  0.8109603724812118   T   T   T
  0.5023775049438370  0.3046490521870098  0.1442937058145404   T   T   T
  0.4976224950561630  0.3046490521870098  0.3557062941854596   T   T   T
  0.4960831747772758  0.3012053567841591  0.6472190815531178   T   T   T
  0.5039168252227242  0.3012053567841591  0.8527809184468822   T   T   T
  0.1705834915089142  0.3012053567841591  0.1861142517802108   T   T   T
  0.1690441712300270  0.3046490521870098  0.4776270391478761   T   T   T
  0.1642891613423529  0.3046490521870098  0.6890396275187882   T   T   T
  0.1627498410634658  0.3012053567841591  0.9805524148864535   T   T   T
  0.6622340912017251  0.4042364695002476  0.1986454882513016   T   T   T
  0.6661988552890747  0.4008889274573235  0.4884453105281850   T   T   T
  0.6671344772833052  0.4008889274573235  0.6782213561384793   T   T   T
  0.6710992413706549  0.4042364695002476  0.9680211784153627   T   T   T
```

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0.3289007586293451	0.4042364695002476	0.5319788215846373	T	T	T
0.3328655227166948	0.4008889274573235	0.8217786438615207	T	T	T
0.9995321890028848	0.4008889274573235	0.1551119771948493	T	T	T
0.0004678109971152	0.4008889274573235	0.3448880228051507	T	T	T
0.0044325750844649	0.4042364695002476	0.6346878450820270	T	T	T
0.9955674249155351	0.4042364695002476	0.8653121549179730	T	T	T
0.1666666662861900	0.1623708975283051	0.0833333333333357	F	F	F
0.8333333337138100	0.1623708971301525	0.4166666666666643	F	F	F
0.5135375913938560	0.1705498330329362	0.0833333333333357	F	F	F
0.1802042588214761	0.1705498326347907	0.4166666666666643	F	F	F
0.4864624074647139	0.1705498326347907	0.4166666666666643	F	F	F
0.3333333337138100	0.0616767845705795	0.4166666666666643	F	F	F
0.1531290737508968	0.1705498330329362	0.7500000000000000	F	F	F
0.5000000000000000	0.1623708975283051	0.7500000000000000	F	F	F
0.8197957411785239	0.1705498326347907	0.0833333333333357	F	F	F
0.6666666674276200	0.0616767849687250	0.0833333333333357	F	F	F
0.8468709251076660	0.1705498326347907	0.7500000000000000	F	F	F
0.0135375925352861	0.0698557200752106	0.0833333333333357	F	F	F
0.3197957400370868	0.0698557200752106	0.0833333333333357	F	F	F
0.6531290748923340	0.1315325046457900	0.2500000000000000	F	F	F
0.3468709251076660	0.1315325050439355	0.2500000000000000	F	F	F
0.0000000000000000	0.1397114401504282	0.2500000000000000	F	F	F
0.6802042588214761	0.0698557200752106	0.4166666666666643	F	F	F
0.9864624074647139	0.0698557200752106	0.4166666666666643	F	F	F
0.3197957400370868	0.1315325046457900	0.5833333333333357	F	F	F
0.0135375925352861	0.1315325050439355	0.5833333333333357	F	F	F
0.6666666662861900	0.1397114401504282	0.5833333333333357	F	F	F
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0.6531290748923340	0.0698557200752106	0.7500000000000000	F	F	F
0.0000000000000000	0.0616767849687250	0.7500000000000000	F	F	F
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0.6802042599629132	0.1315325046457900	0.9166666666666643	F	F	F
0.3333333325723800	0.1397114401504282	0.9166666666666643	F	F	F
0.4999999988585628	0.2404055531081539	0.2500000000000000	F	F	F
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0.5000000000000000	0.3666606025844459	0.7500000000000000	T	T	T
0.4807427483770184	0.4314653499021688	0.9182982364170158	T	T	T
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0.8169327501787436	0.3769986624007871	0.0833092030752240	T	T	T
0.6666666674276200	0.2639771306606633	0.0833333333333357	T	T	T
0.8525905841953616	0.4314653503003214	0.2483684302496485	T	T	T
0.8140760832322655	0.4314653503003214	0.5849649030836872	T	T	T

0.8497339161074464	0.3769986624007871	0.7500241302581117	T	T	T
0.0131697713018397	0.2719301871828037	0.0836331428444410	T	T	T
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0.3465031038742197	0.2719301871828037	0.7502998095111053	T	T	T
0.6534968961257803	0.2719301871828037	0.7497001904888947	T	T	T
0.0000000000000000	0.2639771306606633	0.7500000000000000	T	T	T
0.9850699974062209	0.3321045482886191	0.9183402264987635	T	T	T
0.6815966700214062	0.3321045478904736	0.9149931068345651	T	T	T
0.8333333337138100	0.4396038408219098	0.9166666666666643	T	T	T
0.3333333325723800	0.3379154231103385	0.9166666666666643	T	T	T

(110) surface with one side terminated by hydroxyl groups (Optimized in gas phase):

Title

1.00000000000000

8.7609063200000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 25.1162232400000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.8345004800000009

Fe O H

48 81 18

Selective dynamics

Direct

0.8333333337138100	0.1006941125595731	0.0208726741104570	F	F	F
0.8333333337138100	0.1006941125595731	0.3124606592228787	F	F	F
0.8333333337138100	0.1006941125595731	0.5208726741104570	F	F	F
0.8333333337138100	0.1006941125595731	0.8124606592228787	F	F	F
0.5000000000000000	0.1006941125595731	0.1457939925562073	F	F	F
0.5000000000000000	0.1006941125595731	0.3542060074437927	F	F	F
0.5000000000000000	0.1006941125595731	0.6457939925562073	F	F	F
0.5000000000000000	0.1006941125595731	0.8542060074437927	F	F	F
0.1666666662861900	0.1006941125595731	0.1875393407771213	F	F	F
0.1666666662861900	0.1006941125595731	0.4791273258895430	F	F	F
0.1666666662861900	0.1006941125595731	0.6875393407771213	F	F	F
0.1666666662861900	0.1006941125595731	0.9791273258895430	F	F	F
0.6666666662861900	0.2013882251191532	0.1875393407771213	F	F	F
0.6666666662861900	0.2013882251191532	0.4791273258895430	F	F	F
0.6666666662861900	0.2013882251191532	0.6875393407771213	F	F	F
0.6666666662861900	0.2013882251191532	0.9791273258895430	F	F	F
0.3333333337138100	0.2013882251191532	0.0208726741104570	F	F	F
0.3333333337138100	0.2013882251191532	0.3124606592228787	F	F	F
0.3333333337138100	0.2013882251191532	0.5208726741104570	F	F	F
0.3333333337138100	0.2013882251191532	0.8124606592228787	F	F	F
0.0000000000000000	0.2013882251191532	0.1457939925562073	F	F	F
0.0000000000000000	0.2013882251191532	0.3542060074437927	F	F	F
0.0000000000000000	0.2013882251191532	0.6457939925562073	F	F	F
0.0000000000000000	0.2013882251191532	0.8542060074437927	F	F	F
0.8329665263597372	0.3021716082348493	0.0208682918298217	T	T	T
0.8327471286426709	0.3026944551938156	0.3121661890925559	T	T	T
0.8309228500116853	0.3033439323183072	0.5224874759739019	T	T	T
0.8317275201003059	0.3016707713288326	0.8129991841985892	T	T	T

0.4983802948064384	0.3016787039497829	0.1463202669156479	T	T	T
0.4996295500967016	0.3021724858323039	0.3541952811729754	T	T	T
0.4994349640519575	0.3026867268682478	0.6454967970868499	T	T	T
0.4975941001220954	0.3033405813357401	0.8558407626385219	T	T	T
0.1642343907855217	0.3033543448692703	0.1891538959580609	T	T	T
0.1650684748118843	0.3016863255091383	0.4796393558100104	T	T	T
0.1663029202808443	0.3021545764940151	0.6875173996753301	T	T	T
0.1661168796944697	0.3026954525577581	0.9788283995270245	T	T	T
0.6559660515171123	0.4041576841737404	0.1845183427399965	T	T	T
0.6676598534997191	0.4065821555144840	0.4753249897483315	T	T	T
0.6641920818938080	0.4031292265145235	0.6908155747749479	T	T	T
0.6757498066643288	0.4039932778110567	0.9838324595804129	T	T	T
0.3308265093710099	0.4031631771529809	0.0241179072091853	T	T	T
0.3423888487149659	0.4039919530822372	0.3171774946004413	T	T	T
0.3226514947550738	0.4041557884351755	0.5178500249090100	T	T	T
0.3343728949555085	0.4065642371509851	0.8085869752151733	T	T	T
0.0009934906695383	0.4065937016537499	0.1419664564144811	T	T	T
-0.0025400932855637	0.4031532388132931	0.3574570845746702	T	T	T
0.0090856288436640	0.4039804798267430	0.6505042105662904	T	T	T
0.9893231960950198	0.4041504059762841	0.8512002959488434	T	T	T
0.1666666662861900	0.1623708975283051	0.0833333333333357	F	F	F
0.8333333337138100	0.1623708971301525	0.4166666666666643	F	F	F
0.5135375913938560	0.1705498330329362	0.0833333333333357	F	F	F
0.1802042588214761	0.1705498326347907	0.4166666666666643	F	F	F
0.4864624074647139	0.1705498326347907	0.4166666666666643	F	F	F
0.3333333337138100	0.0616767845705795	0.4166666666666643	F	F	F
0.1531290737508968	0.1705498330329362	0.7500000000000000	F	F	F
0.5000000000000000	0.1623708975283051	0.7500000000000000	F	F	F
0.8197957411785239	0.1705498326347907	0.0833333333333357	F	F	F
0.6666666674276200	0.0616767849687250	0.0833333333333357	F	F	F
0.8468709251076660	0.1705498326347907	0.7500000000000000	F	F	F
0.0135375925352861	0.0698557200752106	0.0833333333333357	F	F	F
0.3197957400370868	0.0698557200752106	0.0833333333333357	F	F	F
0.6531290748923340	0.1315325046457900	0.2500000000000000	F	F	F
0.3468709251076660	0.1315325050439355	0.2500000000000000	F	F	F
0.0000000000000000	0.1397114401504282	0.2500000000000000	F	F	F
0.6802042588214761	0.0698557200752106	0.4166666666666643	F	F	F
0.9864624074647139	0.0698557200752106	0.4166666666666643	F	F	F
0.3197957400370868	0.1315325046457900	0.5833333333333357	F	F	F
0.0135375925352861	0.1315325050439355	0.5833333333333357	F	F	F
0.6666666662861900	0.1397114401504282	0.5833333333333357	F	F	F
0.3468709251076660	0.0698557200752106	0.7500000000000000	F	F	F
0.6531290748923340	0.0698557200752106	0.7500000000000000	F	F	F
0.0000000000000000	0.0616767849687250	0.7500000000000000	F	F	F
0.9864624074647139	0.1315325050439355	0.9166666666666643	F	F	F
0.6802042599629132	0.1315325046457900	0.9166666666666643	F	F	F
0.3333333325723800	0.1397114401504282	0.9166666666666643	F	F	F
0.4999999988585628	0.2404055531081539	0.2500000000000000	F	F	F
0.5135375913938560	0.2322266176035157	0.5833333333333357	F	F	F
0.4864624063232768	0.2322266172053631	0.9166666666666643	F	F	F
0.1802042588214761	0.2322266172053631	0.9166666666666643	F	F	F
0.8468709262491032	0.2322266176035157	0.2500000000000000	F	F	F
0.8197957411785239	0.2322266176035157	0.5833333333333357	F	F	F
0.1531290737508968	0.2322266176035157	0.2500000000000000	F	F	F
0.1666666662861900	0.2404055527100013	0.5833333333333357	F	F	F
0.8333333337138100	0.2404055527100013	0.9166666666666643	F	F	F
0.1657523953224929	0.3643196438505167	0.0849712902357742	T	T	T
0.8324179812268947	0.3643088478657316	0.4183424931726822	T	T	T
0.5126622666251098	0.3710433032145244	0.0823789856987386	T	T	T
0.4863515264979153	0.4429987495104790	0.2393371447084814	T	T	T

0.1793456779218282	0.3710401369317030	0.4157004523767581	T	T	T
0.4879739176193997	0.3733707394177161	0.4158707425873255	T	T	T
0.3334697715744271	0.2630403893701472	0.4172264558674835	T	T	T
0.5094335034914536	0.4325403519572266	0.5850941288542953	T	T	T
0.1546700435626325	0.3733602089301602	0.7491685447981006	T	T	T
0.4991437490491524	0.3642864671451617	0.7516682995261407	T	T	T
0.4871373311133319	0.4330447043819154	0.9187759734618490	T	T	T
0.1762079593744289	0.4325707288428825	0.9183279996102574	T	T	T
0.8213003612871062	0.3733776583612737	0.0825326450372621	T	T	T
0.6668074118630083	0.2630403339916680	0.0839020700716069	T	T	T
0.8427568364775554	0.4325725289535330	0.2517431152558947	T	T	T
0.8204617934938623	0.4330492563657332	0.5855056064509261	T	T	T
0.8460408513384161	0.3710293739483562	0.7490664115020386	T	T	T
0.0131887369529568	0.2716686514443302	0.0835399436557746	T	T	T
0.3182653568078229	0.2713856693180896	0.0835359967937662	T	T	T
0.1538026757973722	0.4330520613353829	0.2521426792028091	T	T	T
0.6520146881123606	0.3340857994766308	0.2502144084381564	T	T	T
0.3461258680509808	0.3333656518423595	0.2511452492159703	T	T	T
0.9978054811381634	0.3429179593224315	0.2503831967688551	T	T	T
0.6798721277542085	0.2716643723218161	0.4168640262505452	T	T	T
0.9849526176842278	0.2713869947767606	0.4168632192314436	T	T	T
0.3187141066683157	0.3340816796218209	0.5835445241854325	T	T	T
0.0128061591727827	0.3333649429120961	0.5844690477376824	T	T	T
0.1530407373063711	0.4429874241686573	0.5726718225448690	T	T	T
0.6645130396146982	0.3429065422783041	0.5837368394235144	T	T	T
0.3465420525534552	0.2716599198825573	0.7502001082771932	T	T	T
0.6516382550106419	0.2713820380964005	0.7502020907015953	T	T	T
0.0001391276050878	0.2630348274561393	0.7505653929509037	T	T	T
0.9853838441309516	0.3340866581416522	0.9168974825048795	T	T	T
0.6794822134706849	0.3333649049233601	0.9178104598454779	T	T	T
0.8197247432464628	0.4429974815738312	0.9060002692602861	T	T	T
0.3311768217775778	0.3429053029012417	0.9170578321171741	T	T	T
0.6878392089881434	0.4757650159834800	0.4232460170398066	T	T	T
0.6762522157119766	0.4725939086058836	0.7519575877096987	T	T	T
0.3429715619574846	0.4726225411383573	0.0852741416593879	T	T	T
0.3546018236174039	0.4757610687474906	0.7565175056524747	T	T	T
0.0094522052827823	0.4725853151404209	0.4186481025632444	T	T	T
0.0213511382834664	0.4757930260088155	0.0899598089487495	T	T	T
0.6741787237676174	0.4637278357110365	0.0842596787309437	T	T	T
0.3409288181219042	0.4637363083998123	0.4176147106999889	T	T	T
0.0076466683438926	0.4637232282021293	0.7509600558142155	T	T	T
0.8295920873166071	0.4708894549661975	0.2603491397127251	T	T	T
0.7589617862274930	0.4593166174093326	0.8493775358975640	T	T	T
0.4256402920803698	0.4593248004350622	0.1827578013882910	T	T	T
0.4963544485147073	0.4708613499393792	0.5937081316969620	T	T	T
0.0922145647690675	0.4593029501793121	0.5160347858711917	T	T	T
0.5906940440669098	0.4893130571773788	0.3986982633331808	T	T	T
0.5730974704705153	0.4878854652038725	0.7576438636745059	T	T	T
0.2398319601786912	0.4879392092145960	0.0908481318416165	T	T	T
0.2575384722874300	0.4892845357890256	0.7317998910471416	T	T	T
0.9062657622458031	0.4878491307396033	0.4243724733446728	T	T	T
0.1634697024463639	0.4709343130800387	0.9264696273854128	T	T	T
0.9243081776475376	0.4893994943172532	0.0653773078092928	T	T	T
0.4811775155887603	0.4718565627255250	0.9182573285507134	T	T	T
0.9143161621848589	0.4851743308973175	0.7498104963730955	T	T	T
0.8144563521294683	0.4718597696472754	0.5850600747334672	T	T	T
0.2475932278064197	0.4851856390132668	0.4164469067825568	T	T	T
0.1478808189253936	0.4718638260645881	0.2514225452490009	T	T	T
0.5807304676907675	0.4851201223789224	0.0830660421302138	T	T	T

(110) surface with one side terminated by hydroxyl groups (Optimized in dielectric medium):

```
Title
   1.00000000000000
     8.7609063200000001    0.0000000000000000    0.0000000000000000
     0.0000000000000000   25.1162232400000001    0.0000000000000000
     0.0000000000000000    0.0000000000000000   13.8345004800000009
   Fe   O    H
    48   81   18
Selective dynamics
Direct
  0.8333333337138100  0.1006941125595731  0.0208726741104570   F   F   F
  0.8333333337138100  0.1006941125595731  0.3124606592228787   F   F   F
  0.8333333337138100  0.1006941125595731  0.5208726741104570   F   F   F
  0.8333333337138100  0.1006941125595731  0.8124606592228787   F   F   F
  0.5000000000000000  0.1006941125595731  0.1457939925562073   F   F   F
  0.5000000000000000  0.1006941125595731  0.3542060074437927   F   F   F
  0.5000000000000000  0.1006941125595731  0.6457939925562073   F   F   F
  0.5000000000000000  0.1006941125595731  0.8542060074437927   F   F   F
  0.1666666662861900  0.1006941125595731  0.1875393407771213   F   F   F
  0.1666666662861900  0.1006941125595731  0.4791273258895430   F   F   F
  0.1666666662861900  0.1006941125595731  0.6875393407771213   F   F   F
  0.1666666662861900  0.1006941125595731  0.9791273258895430   F   F   F
  0.6666666662861900  0.2013882251191532  0.1875393407771213   F   F   F
  0.6666666662861900  0.2013882251191532  0.4791273258895430   F   F   F
  0.6666666662861900  0.2013882251191532  0.6875393407771213   F   F   F
  0.6666666662861900  0.2013882251191532  0.9791273258895430   F   F   F
  0.3333333337138100  0.2013882251191532  0.0208726741104570   F   F   F
  0.3333333337138100  0.2013882251191532  0.3124606592228787   F   F   F
  0.3333333337138100  0.2013882251191532  0.5208726741104570   F   F   F
  0.3333333337138100  0.2013882251191532  0.8124606592228787   F   F   F
  0.0000000000000000  0.2013882251191532  0.1457939925562073   F   F   F
  0.0000000000000000  0.2013882251191532  0.3542060074437927   F   F   F
  0.0000000000000000  0.2013882251191532  0.6457939925562073   F   F   F
  0.0000000000000000  0.2013882251191532  0.8542060074437927   F   F   F
  0.8331295855503600  0.3018908353742187  0.0206937068097354   T   T   T
  0.8328626033047704  0.3024904533331249  0.3120115886849780   T   T   T
  0.8316513009198248  0.3028685693812272  0.5220649479725168   T   T   T
  0.8319642892376198  0.3014902270911057  0.8129429912031665   T   T   T
  0.4986296782967262  0.3014915468782361  0.1462826141772796   T   T   T
  0.4998100394030354  0.3018925029781680  0.3540256878875077   T   T   T
  0.4995310492213619  0.3024925200505307  0.6453466627389224   T   T   T
  0.4983101028910306  0.3028686790389020  0.8553969910912984   T   T   T
  0.1649736966894887  0.3028726454746768  0.1887348841315117   T   T   T
  0.1653129936929902  0.3014910748567058  0.4796034982535109   T   T   T
  0.1664651669668614  0.3018920756611687  0.6873571313348058   T   T   T
  0.1661978928067241  0.3024897526776046  0.9786821145317306   T   T   T
  0.6570218038106175  0.4039235677542564  0.1844882611027090   T   T   T
  0.6685720046380927  0.4054678901078052  0.4762562804969126   T   T   T
  0.6645659068407430  0.4029293687678692  0.6902909390987468   T   T   T
  0.6750667272434283  0.4034141424586021  0.9838982317952760   T   T   T
  0.3312391506952831  0.4029246468069795  0.0236334724958872   T   T   T
  0.3417448231226116  0.4034164394682492  0.3172285890103528   T   T   T
  0.3236784753041281  0.4039247706095517  0.5178272382187283   T   T   T
  0.3352402671195748  0.4054726141272013  0.8095981763654027   T   T   T
  0.0019073733631997  0.4054715653445956  0.1429262253103830   T   T   T
  0.9978912177382125  0.4029342042628411  0.3569656047600139   T   T   T
  0.0084059313278056  0.4034157152719996  0.6505600036459315   T   T   T
  0.9903397427075349  0.4039200714220922  0.8511489411179285   T   T   T
  0.1666666662861900  0.1623708975283051  0.0833333333333357   F   F   F
```

0.8333333337138100	0.1623708971301525	0.4166666666666643	F	F	F
0.5135375913938560	0.1705498330329362	0.0833333333333357	F	F	F
0.1802042588214761	0.1705498326347907	0.4166666666666643	F	F	F
0.4864624074647139	0.1705498326347907	0.4166666666666643	F	F	F
0.3333333337138100	0.0616767845705795	0.4166666666666643	F	F	F
0.1531290737508968	0.1705498330329362	0.7500000000000000	F	F	F
0.5000000000000000	0.1623708975283051	0.7500000000000000	F	F	F
0.8197957411785239	0.1705498326347907	0.0833333333333357	F	F	F
0.6666666674276200	0.0616767849687250	0.0833333333333357	F	F	F
0.8468709251076660	0.1705498326347907	0.7500000000000000	F	F	F
0.0135375925352861	0.0698557200752106	0.0833333333333357	F	F	F
0.3197957400370868	0.0698557200752106	0.0833333333333357	F	F	F
0.6531290748923340	0.1315325046457900	0.2500000000000000	F	F	F
0.3468709251076660	0.1315325050439355	0.2500000000000000	F	F	F
0.0000000000000000	0.1397114401504282	0.2500000000000000	F	F	F
0.6802042588214761	0.0698557200752106	0.4166666666666643	F	F	F
0.9864624074647139	0.0698557200752106	0.4166666666666643	F	F	F
0.3197957400370868	0.1315325046457900	0.5833333333333357	F	F	F
0.0135375925352861	0.1315325050439355	0.5833333333333357	F	F	F
0.6666666662861900	0.1397114401504282	0.5833333333333357	F	F	F
0.3468709251076660	0.0698557200752106	0.7500000000000000	F	F	F
0.6531290748923340	0.0698557200752106	0.7500000000000000	F	F	F
0.0000000000000000	0.0616767849687250	0.7500000000000000	F	F	F
0.9864624074647139	0.1315325050439355	0.9166666666666643	F	F	F
0.6802042599629132	0.1315325046457900	0.9166666666666643	F	F	F
0.3333333325723800	0.1397114401504282	0.9166666666666643	F	F	F
0.4999999988585628	0.2404055531081539	0.2500000000000000	F	F	F
0.5135375913938560	0.2322266176035157	0.5833333333333357	F	F	F
0.4864624063232768	0.2322266172053631	0.9166666666666643	F	F	F
0.1802042588214761	0.2322266172053631	0.9166666666666643	F	F	F
0.8468709262491032	0.2322266176035157	0.2500000000000000	F	F	F
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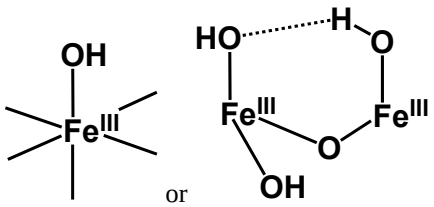

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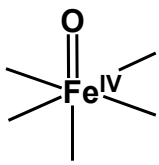

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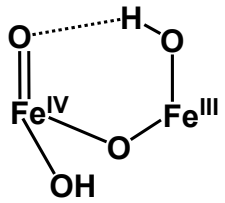

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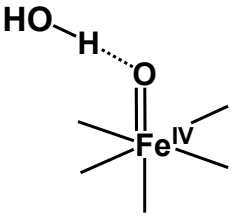

A water molecule hydrogen binding to Intermediate **II**:

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0.0000000000000000 0.2013882251191532 0.8542060074437927 F F F
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0.1652621747793079 0.3029943457579239 0.1888125443289608 T T T
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0.6572514706577501 0.4046577182711708 0.1850199108142301 T T T
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0.6664664056443350 0.4037041756834189 0.6914176191096381 T T T
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0.3321131910481460 0.4027342891179996 0.0228538359255046 T T T

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0.8274295837921954	0.0404427692131009	0.9165220391101556	F	F	F
0.1604631231806195	0.0404836766373649	0.5831760800950860	F	F	F
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0.8099082652900691	0.0287527556631133	0.5759669285869293	F	F	F
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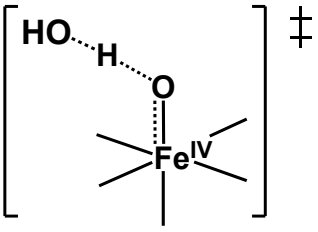

Transition state of H-abstraction (**TS$_{II-III}$**):

Title
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0.0000000000000000 25.1162232400000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.8345004800000009
Fe O H
48 91 37
Selective dynamics
Direct
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0.8343569999999971 0.1012330000000006 0.3102179999999989 F F F
0.8301999999999978 0.0983000000000018 0.5238769999999987 F F F
0.8412000000000006 0.0999290000000030 0.8158699999999967 F F F
0.5076120000000017 0.0999880000000033 0.1491460000000017 F F F
0.4904750000000035 0.1002760000000009 0.3502489999999980 F F F
0.5010440000000003 0.1012350000000026 0.6437740000000004 F F F
0.4964050000000028 0.0982839999999996 0.8574770000000027 F F F
0.1632419999999968 0.0983050000000034 0.1906620000000032 F F F
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0.9987819829709930	0.4029196880675341	0.3562467405948726	T	T	T
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0.3451220000000035	0.0609439999999992	0.4273749999999977	F	F	F
0.1531289999999998	0.1705499999999986	0.7499999999999999	F	F	F
0.5000000000000000	0.1623710000000003	0.7499999999999999	F	F	F
0.8197959999999966	0.1705499999999986	0.0833330000000032	F	F	F
0.6765899999999974	0.0605589999999978	0.0932409999999990	F	F	F
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0.3326660000000032	0.1398330000000030	0.9160090000000024	F	F	F
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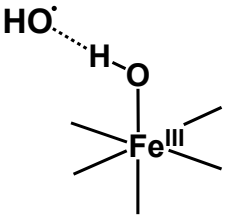

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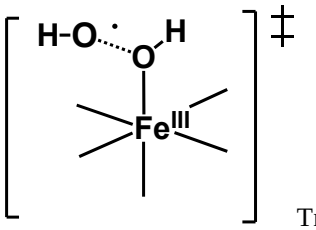

Transition state of H-abstraction (**TS$_{III\text{-}IV}$**):

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Fe O H
48 91 37
Selective dynamics

Direct

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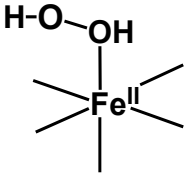

Intermediate **IV**:

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Fe O H
48 91 37
Selective dynamics
Direct

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0.4964049404422823	0.0982838417389402	0.8574768403925788	F	F	F
0.1632416804566432	0.0983050427768077	0.1906616522810651	F	F	F
0.1749643854198837	0.0998813781048398	0.4823784392972925	F	F	F
0.1570696169708583	0.1002621359882454	0.6834783716021846	F	F	F
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0.6666666662861900	0.2013882251191532	0.6875393407771213	F	F	F
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0.8274295837921954	0.0404427692131009	0.9165220391101556	F	F	F
0.1604631231806195	0.0404836766373649	0.5831760800950860	F	F	F
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0.8099082652900691	0.0287527556631133	0.5759669285869293	F	F	F
0.1443634669523561	0.0286502780742097	0.2424324994493787	F	F	F
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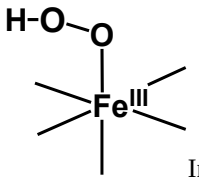

Intermediate **V**:

Title
1.00000000000000
8.7609063200000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 25.1162232400000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.8345004800000009
Fe O H
48 91 36
Selective dynamics
Direct

0.8233502729658255	0.1001473671405364	0.0169663755001039	F	F	F
0.8343567278322439	0.1012329602943893	0.3102183375687702	F	F	F
0.8301996305332011	0.0983002251735030	0.5238772900024529	F	F	F
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0.4904749375290649	0.1002762296677204	0.3502488504738537	F	F	F
0.5010442675296147	0.1012348996783317	0.6437741155074903	F	F	F
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0.1632416804566432	0.0983050427768077	0.1906616522810651	F	F	F
0.1749643854198837	0.0998813781048398	0.4823784392972925	F	F	F
0.1570696169708583	0.1002621359882454	0.6834783716021846	F	F	F
0.1673315541171121	0.1012109820696097	0.9768824295129122	F	F	F
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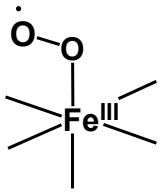

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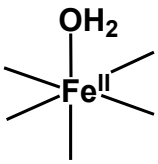

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48 90 37
Selective dynamics
Direct

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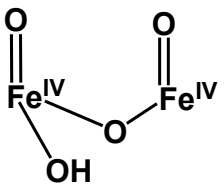

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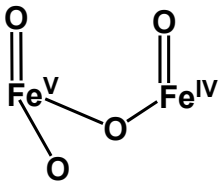

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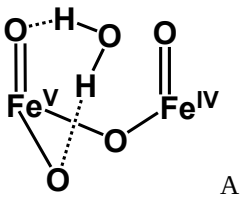

A water molecule hydrogen binding to Intermediate **D**:

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Fe O H
48 91 35
Selective dynamics
Direct

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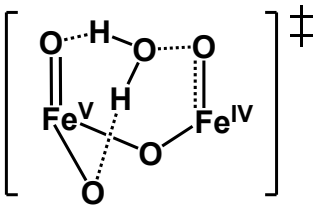

Transition state of water nucleophilic attack (**TS$_{D\text{-}E}$**):

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0.0000000000000000 25.1162232400000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.8345004800000009
Fe O H
48 91 35
Selective dynamics
Direct
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0.5010440004339642 0.1012350000118900 0.6437739998546020 F F F
0.4964049997968729 0.0982839998041029 0.8574770001381322 F F F
0.1632420000582755 0.0983050001748609 0.1906619999625718 F F F
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0.1570700004928227 0.1002619998212779 0.6834780000672607 F F F
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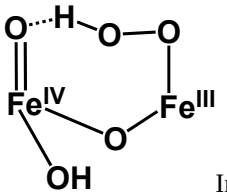

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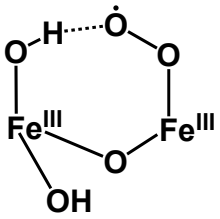

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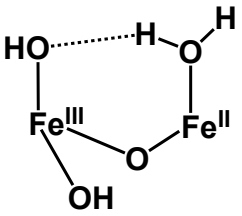

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