

Supporting information for:

Enhanced Electrochemical Water Oxidation: The Impact of Nano-clusters and Nano-cavities

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The plane wave energy cutoff of 600 eV was used in the calculations. Ion positions were relaxed using the conjugate gradient method and the stopping criterion for the ionic relaxation was chosen for all forces (for the relaxed atoms) to be smaller than 3×10^{-2} eV/Å. The stopping criterion for relaxation of the electronic degrees of freedom was chosen for energy change between two steps to be smaller than 10^{-4} . The standard atomic PAW potentials were used: H (valence: 1s), O (valence: 2s2p), and Fe (valence: 3p3d4s). In the calculations of free energy changes, we use previously reported values for $\Delta\text{ZPE} - T\Delta\text{S}$,¹ since they were found earlier very similar between different oxide materials.² The values used are, 0.4, -0.39, 0.47 eV for the formation of O, OH, OOH respectively, and $\Delta G_{(2\text{H}_2\text{O} \rightarrow \text{O}_2 + 2\text{H}_2)} = 4.92$ eV. Energies of non-adsorbed species were previously calculated in the literature: -6.77 eV, -9.87 eV, and -14.22 eV for H₂, O₂, and H₂O, respectively.^{1, 3} The converged k-grid of $2 \times 2 \times 1$ was used for the hematite slabs. For the WO₃ slabs, the k-grid of $4 \times 4 \times 1$ was used.

Figure S1 shows the atomic distances between the neighboring Fe atoms. It is too complicated to assign a Fe atom as the first (or second) neighbour due to very diverse Fe-Fe distances.

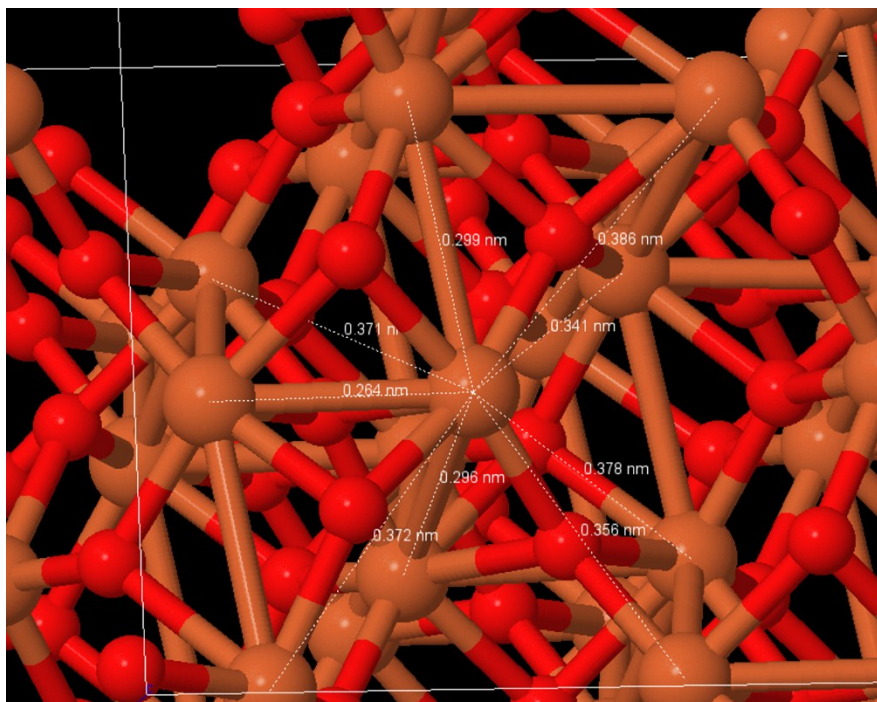


Figure S1. Distances between Fe-Fe atoms.

1. P. Liao, J. A. Keith and E. A. Carter, *J. Am. Chem. Soc.*, 2012, **134**, 13296-13309.
2. D. K. Kanan, J. A. Keith and E. A. Carter, *ChemElectroChem*, 2014, **1**, 407-415.
3. O. Neufeld and M. C. Toroker, *The Journal of Physical Chemistry C*, 2015, **119**, 5836-5847.

Coordinates

The geometries are given according to the following order: title, lattice vectors in Cartesian coordinates, atom types, number of atoms, and atom positions in fractional coordinates with respect to the lattice vectors (with the last Fe-O layer fixed), respectively.

```
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0.00000000000000020 0.00000000000000000 24.3497499999999718
O Fe
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O Fe

118 58

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