Supporting information:

Why does NiOOH cocatalyst increase the oxygen evolution activity of α-Fe_2O_3?

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Slabs and geometries

Different geometries of NiOOH on Fe_2O_3 were used in this study: the cluster, the strip, and the wider strip geometry. Different slab sizes were used depending on the geometry. In each case, the NiOOH layer and the Fe_2O_3 slab were first optimized separately. The relaxed structures were then optimized together. These finally relaxed geometries are shown in Figure S1 in top view representation. There is a vacuum of 9 Å in the z direction for all geometries.

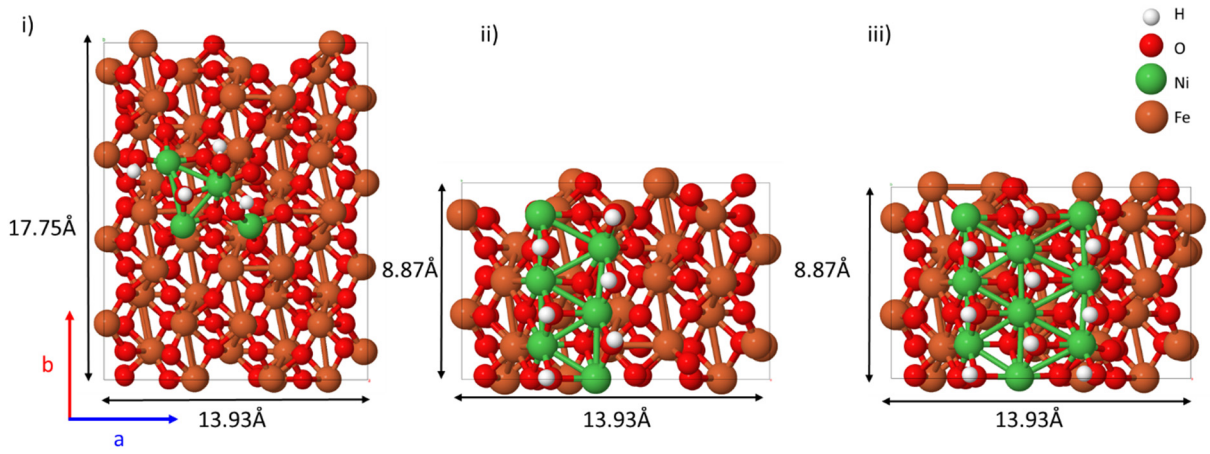

Figure S1 Top views of the slabs of NiOOH on Fe_2O_3 of the three different geometries used in this study i) cluster, ii) strip, and iii) wider strip geometries. All geometries are the final geometries after optimization.

Reconstructions in cluster geometry during OER at the terminal site

The cluster geometry shows reconstructions when it is optimized with adsorbed OER intermediates. Figure S2 shows the reconstructions observed in the cluster geometry during adsorption of OER intermediates at the terminal site.

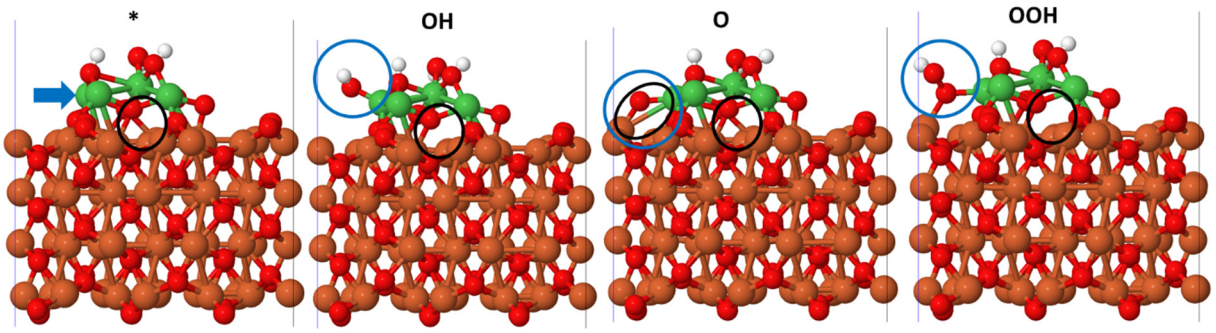

Figure S2 Side views of geometries showing OER intermediates adsorbed at the terminal site of the cluster (blue circle). The reconstructions in these geometries after optimization are marked by the black circles.

Lattice mismatch

Due to different lattice constants of NiOOH and Fe_2O_3, it is important to check for lattice mismatch in the optimized geometries. In the case of geometry *ii* and *iii* (Figure S2), the length of the hematite slab in *b* direction is 8.87 Å and the length of the NiOOH strip in *b* direction is 8.44 Å before optimization. Hence, there is a lattice mismatch of 4.84% ((8.87 Å - 8.44 Å)/8.87 Å) between the hematite slab and NiOOH strip before optimization. The full cell was optimized and after optimization, the NiOOH strip relaxed over the hematite slab to match the *b* dimension of 8.87 Å. This results in a final optimized geometry without lattice mismatch.

Calculation of ΔG for OER intermediates

From Kanan et al., the ΔZPE - TΔS values are found to be similar for OER at different oxide materials.[1] Hence, previously reported values for ΔZPE – TΔS were used in this paper for the calculations of free energy changes.[2] The values are 0.4 eV, -0.39 eV, and 0.47 eV for the formation of OH, O, OOH, respectively, and 4.92 eV for ΔG ($2H_2O \rightarrow O_2 + 2H_2$).[2] Energies of non-adsorbed species, i.e. H_2, O_2, and H_2O, were also derived from the literature: the values are −6.77 eV, −9.87 eV, and −14.22 eV, respectively.[2,3]

Adsorption induced reconstructions in two atom wide geometry

The Ni-Fe bond lengths in different geometries (A, B, C site) with adsorbed OH are compared against the optimized geometry without any adsorbed species (*) in Figure S3. The bond length changes in all three geometries: 0.322 nm for A site, 0.305 nm for B site, and 0.317 nm for C site vs 0.326 nm for plain geometry. This indicates that the two atom wide geometry is not stable enough. The B site adsorption results in the highest displacement compared to the A site and the C site.

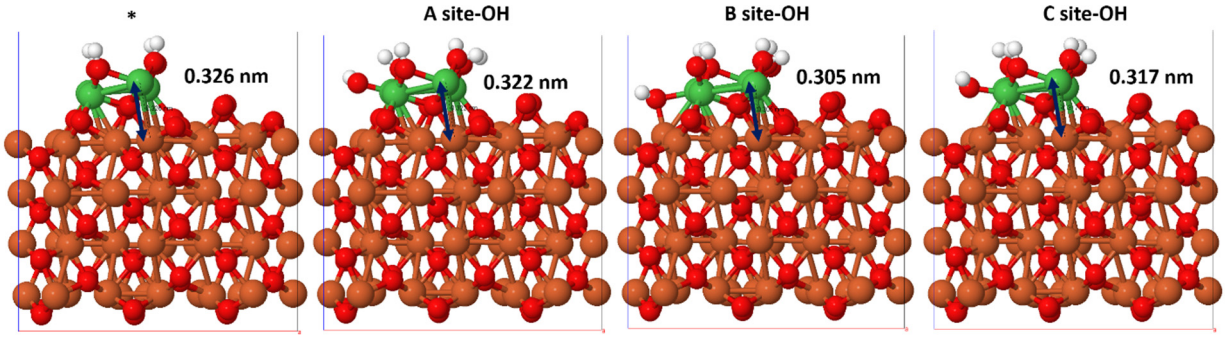

Figure S3 Side views of geometries showing the relaxed two atom wide geometry and geometries with OH adsorbed at A, B, and C sites. An Fe-Ni bond length on the non-adsorbing side is chosen as reference (black arrow) to show the displacement of the cocatalyst layer with respect to the hematite surface.

Adsorption on wider strip geometry

The wider strip geometries are analyzed similar to the two atom wide geometry above (Figure S4). In this case after adsorption of species at A, B, and C sites, the bond lengths remain approximately same, unlike the two atom wide geometry. Hence, the three atom wide geometry does not show any adsorption induced reconstructions and is stable.

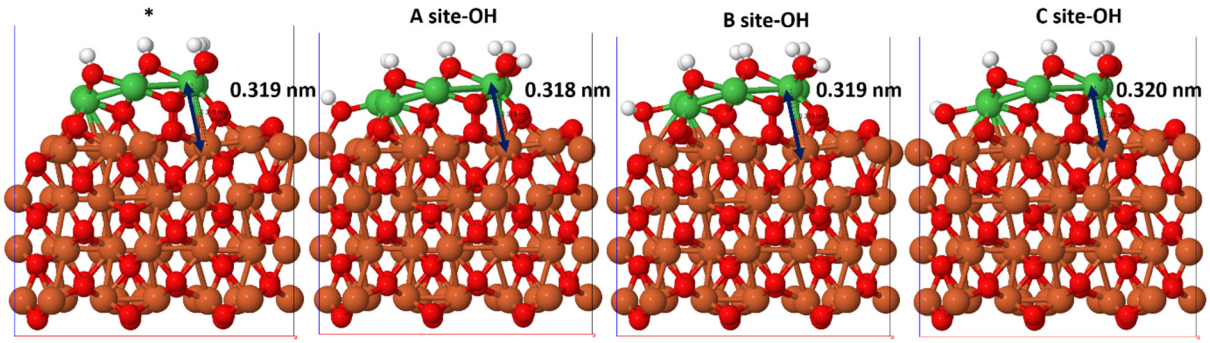

Figure S4 Side views of geometries showing the relaxed wider strip geometry and geometries with OH adsorbed at A, B and C sites. An Fe-Ni bond length on the non-adsorbing side is chosen as reference (black arrow) to show the displacement of the cocatalyst layer with respect to the hematite surface.

References

1. Kanan, D. K., Keith, J. A. & Carter, E. A. First-Principles Modeling of Electrochemical Water Oxidation on MnO:ZnO(001). *ChemElectroChem* **1,** 407–415

2. Liao, P., Keith, J. A. & Carter, E. A. Water oxidation on pure and doped hematite (0001) surfaces: Prediction of Co and Ni as effective dopants for electrocatalysis. *J. Am. Chem. Soc.* **134,** 13296–13309 (2012).

3. Neufeld, O. & Toroker, M. C. Platinum-Doped α-Fe2O3 for Enhanced Water Splitting Efficiency: A DFT+U Study. *J. Phys. Chem. C* **119,** 5836–5847 (2015).

Lattice parameters and coordinates:

The lattice parameters and coordinates for each of the geometries given in Fig S1 are attached.

i) Cluster geometry

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ii) Strip geometry

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0.0000000000000000 8.8780445411610920 0.0000000000000070

0.0000000000000000 0.0000000000000000 22.0318796272960853

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iii) Wider strip geometry

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