Supporting information for

Atomic-Scale Structure of the Hematite α-$Fe_2O_3(1\bar{1}02)$ "R-cut" Surface

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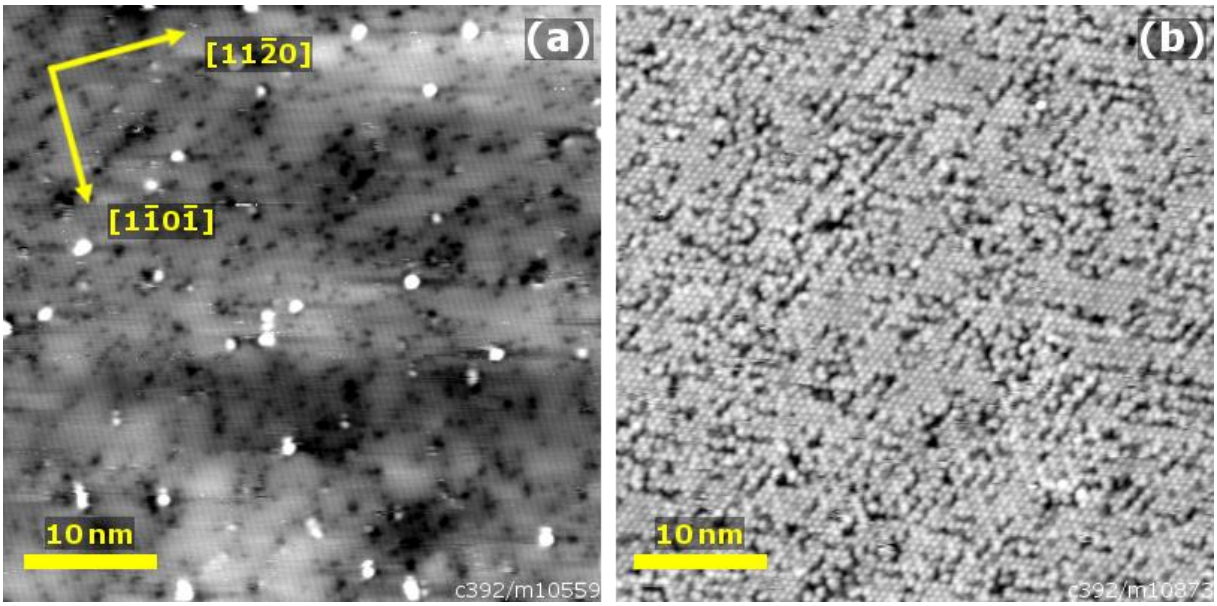

Figure S1: Larger-area STM images of the α-$Fe_2O_3(1\bar{1}02)$ surface with (a) (1×1) termination (45×45 nm^2, U_{sample} = +3 V, I_{tunnel} = 0.1 nA) and (b) (2×1) termination (45×45 nm^2, U_{sample} = -3 V, I_{tunnel} = 0.1 nA).

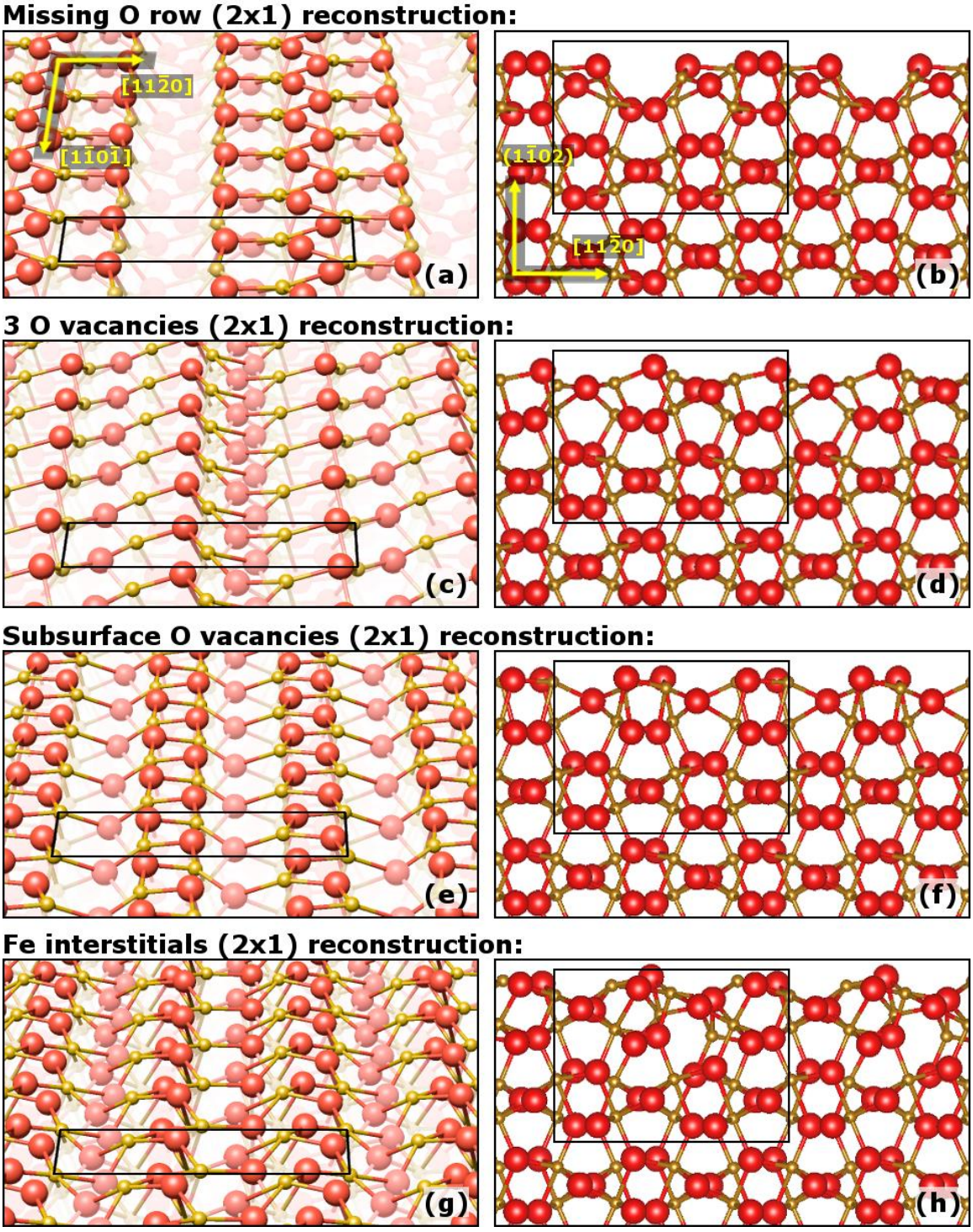

Figure S2: Minimum-energy configurations for (2×1) reconstruction models found to be energetically unfavourable, shown as dashed lines in Fig. 9. Panels (a,b) show a reconstruction model with every other layer-1 oxygen zigzag row removed, as suggested in ref. 1. The model shown in (c,d) is based on the alternating trench model (Fig. 10 (e,f)), with one additional layer-3 oxygen atom removed per (2×1) unit cell. The subsurface oxygen vacancy model in (e,f) is constructed in a similar fashion as the alternating trench model, but with oxygen removed from layer 3 instead of layer 1. Finally, (g,h) shows a model where one iron interstitial per (2×1) unit cell was introduced below layer 5.

The (1×1) and alternating trench (2×1) models in CIF file format are provided as separate files, which were created using VESTA.[2]

References

1. Henderson, M. A., Low Temperature Oxidation of Fe^{2+} Surface Sites on the (2×1) Reconstructed Surface of α-Fe_2O_3 (01$\bar{1}$2). *Surf. Sci.* **2010**, *604*, 1197-1201.
2. Momma, K.; Izumi, F., VESTA 3 for Three-Dimensional Visualization of Crystal, Volumetric and Morphology Data. *J. Appl. Crystallogr.* **2011**, *44*, 1272-1276.