Supporting information for manuscript

Reactivity of sub 1nm supported clusters: $(TiO_2)_n$ clusters supported on rutile TiO_2 (110)

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The supporting information for this manuscript is four figures: S1 to S4.

Figures S1 and S2 show the DFT and DFT+U (U = 4.5 eV in Ti 3d states) spin density plots for oxygen vacancy structures for supported Ti_2O_4 (figure S1) and Ti_4O_8 (figure S2)

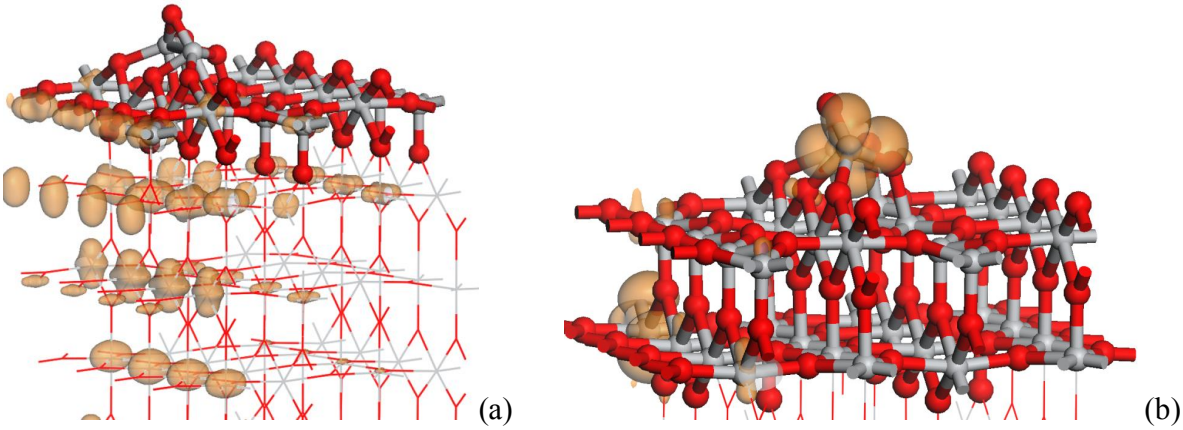

Figure S1: Comparison of DFT and DFT+U spin density for oxygen vacancy structures for Ti_2O_4 and supported on TiO_2. (a): DFT, (b): DFT+U, as described in the text. Different slab thicknesses are shown to highlight the DFT delocalisation

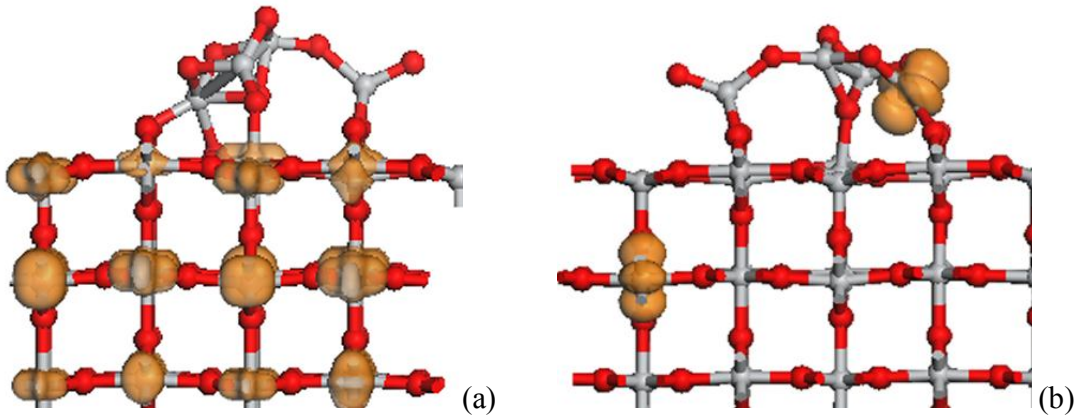

Figure S2: Comparison of DFT and DFT+U spin density for oxygen vacancy structures for Ti_4O_8 and supported on TiO_2. (a): DFT, (b): DFT+U, as described in the text. Different slab thicknesses are shown to highlight the DFT delocalisation

Figure S3 shows the relaxed structures for oxygen vacancy sites 2 and 4 in supported Ti_3O_6

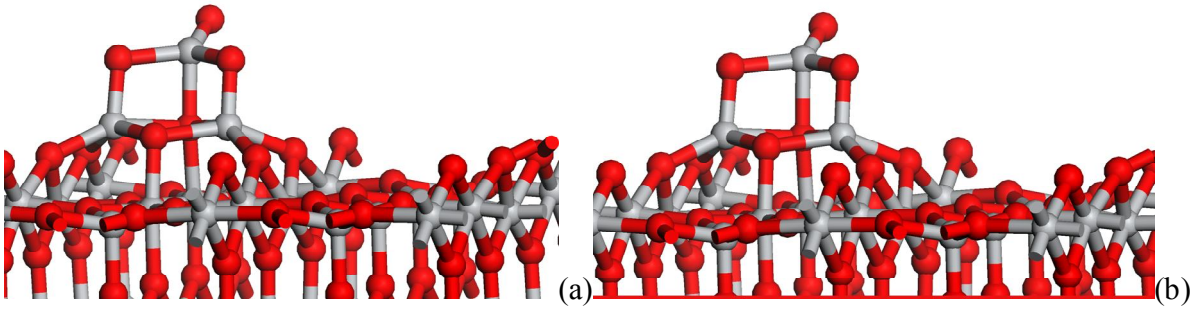

Figure S3: Relaxed atomic structures for oxygen vacancy sites 2 and 4 in reduced Ti_3O_6 supported on TiO_2. (a): site 2, (b): site 4

Figure S4 shows the relaxed structures for oxygen vacancy sites 1 and 2 in supported Ti_4O_8

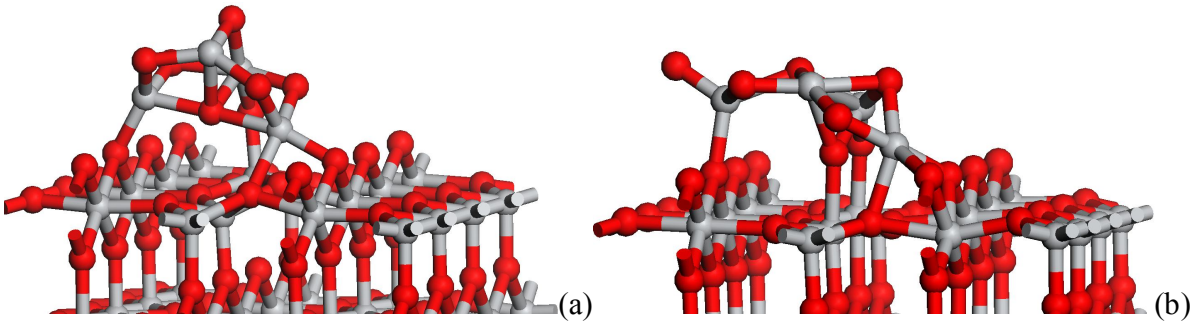

Figure S4: Relaxed atomic structures for oxygen vacancy sites 1 and 2 in reduced Ti_4O_7 supported on TiO_2. (a): site 1, (b): site 2