

Electronic Supplementary Information

Crystal properties without crystallinity? How surface hydroxylation affects the structure and properties of TiO₂ nanoparticles

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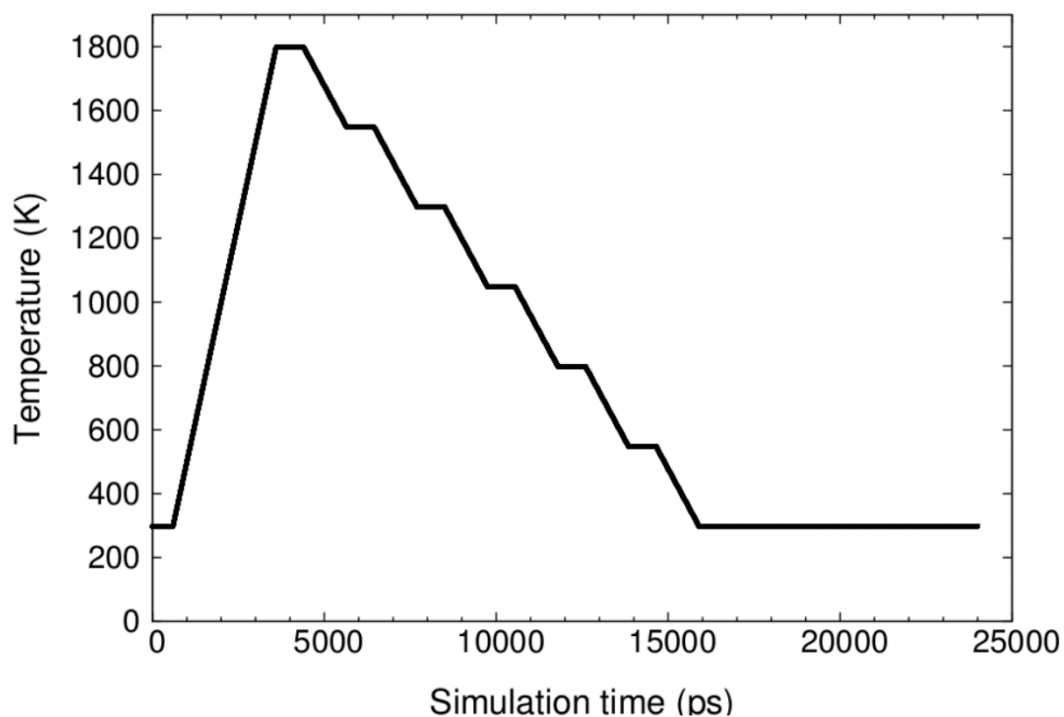


Fig. S1 Temperature evolution profile followed during the stepwise molecular dynamics simulated annealing (MD-SA) procedure.

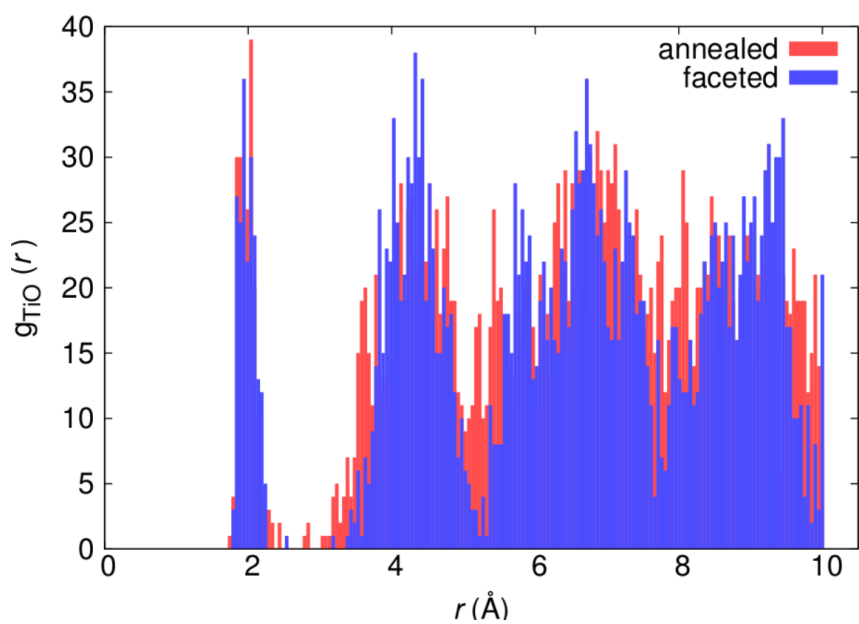


Fig. S2 Pair distribution function, $g(r)$, for Ti-O distances in a faceted crystalline anatase NP (blue) and thermally annealed NP (red) with a $(\text{TiO}_2)_{35}(\text{H}_2\text{O})_{25}$ composition. The bin size for the histogram is 0.05 Å.

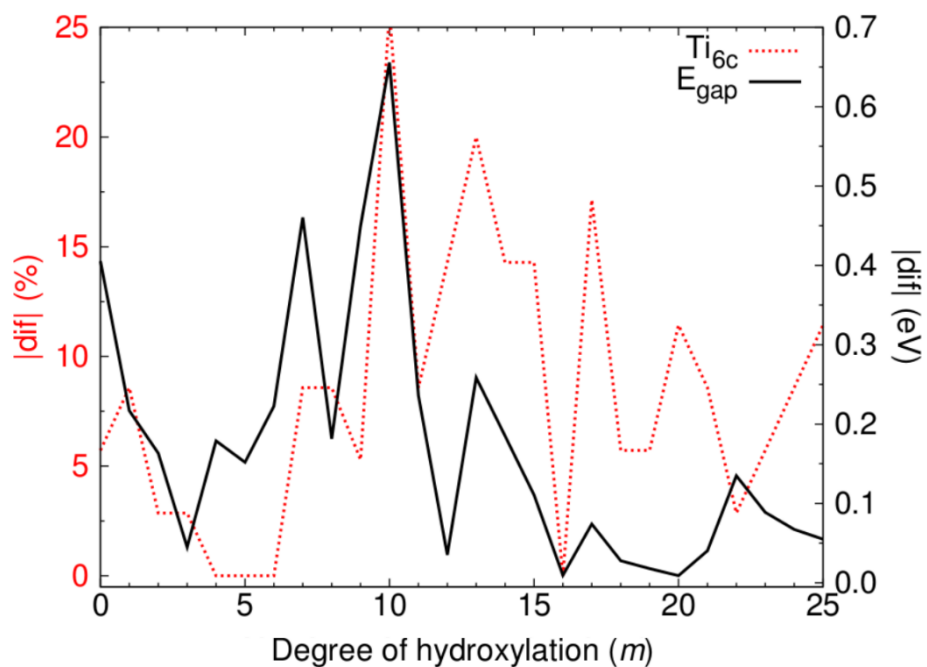


Fig. S3 Difference in the proportion of Ti_{6c} centres (left) and E_{gap} (right) between the crystalline anatase and annealed $(\text{TiO}_2)_{35}(\text{H}_2\text{O})_m$ NPs.