Supplementary Information

Hydrogen Treated Anatase TiO_2: A New Experimental Approach and Further Insights from Theory

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Electronic structure of V_O and H_O defects calculated with the HSE06 functional

We performed additional calculations of the density of states for the 3×3×1 supercell of anatase TiO_2 containing V_O and H_O defects using the hybrid functional HSE06 within the Vienna ab initio Simulation Package (VASP)[1-3]. In detail the defect-free supercell and the supercells containing 1 and 6 defects (corresponding to defect concentrations of 1.4% and 8.3%) are considered. Compared to the PBE+U calculations in the main text a reduced 2×2×2 k-point sampling was used in order to keep the hybrid functional computations feasible. We obtain good qualitative agreement to the PBE+U results as detailed in the main text, see Fig. S2 and Fig. 9.

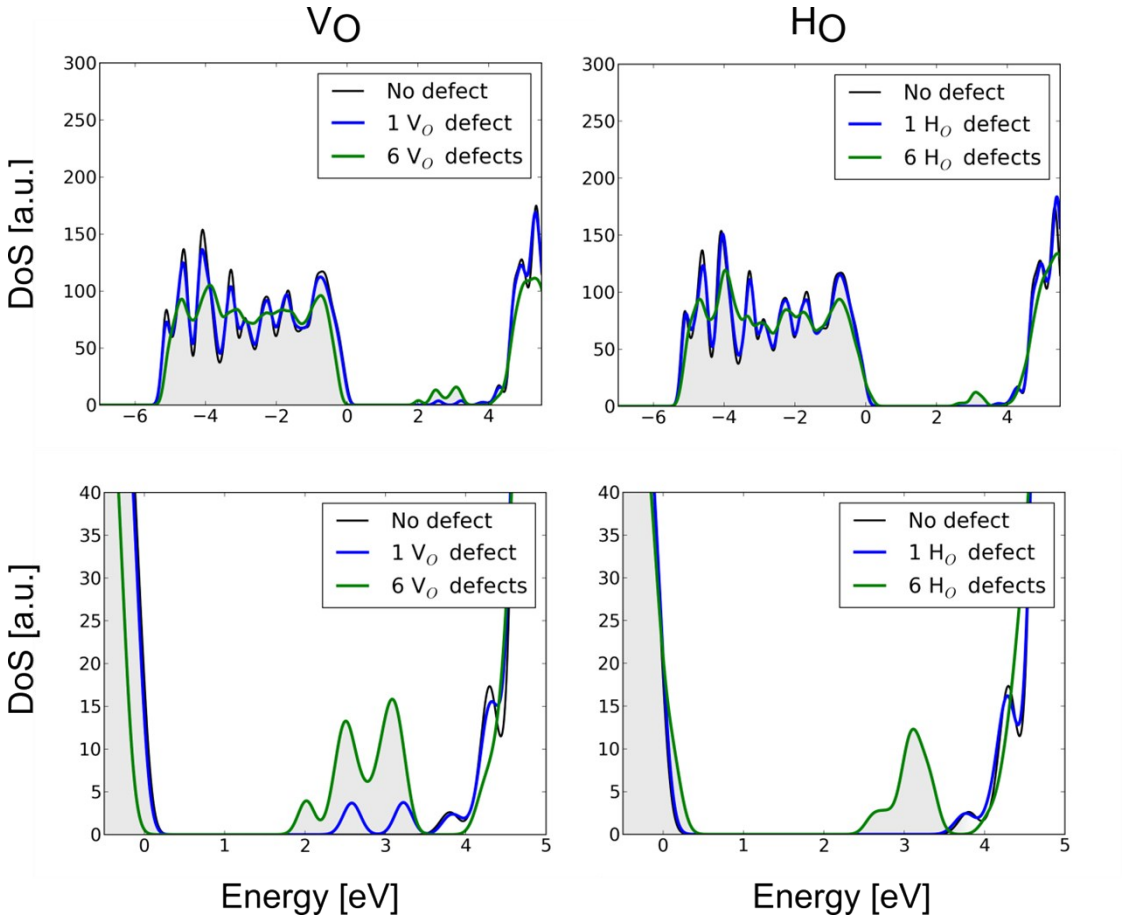

Fig. S1 Density of states (DoS) of anatase TiO_2 with different concentrations of oxygen vacancies V_O on the left and substitutional H_O defects on the right side. The band gap areas are enlarged in the bottom panels. The highest occupied state of pristine TiO_2 sets the zero energy. Occupied energy levels are indicated by the grey shading. See Fig. S2 for the alignment of the energy levels in the presence of defects.

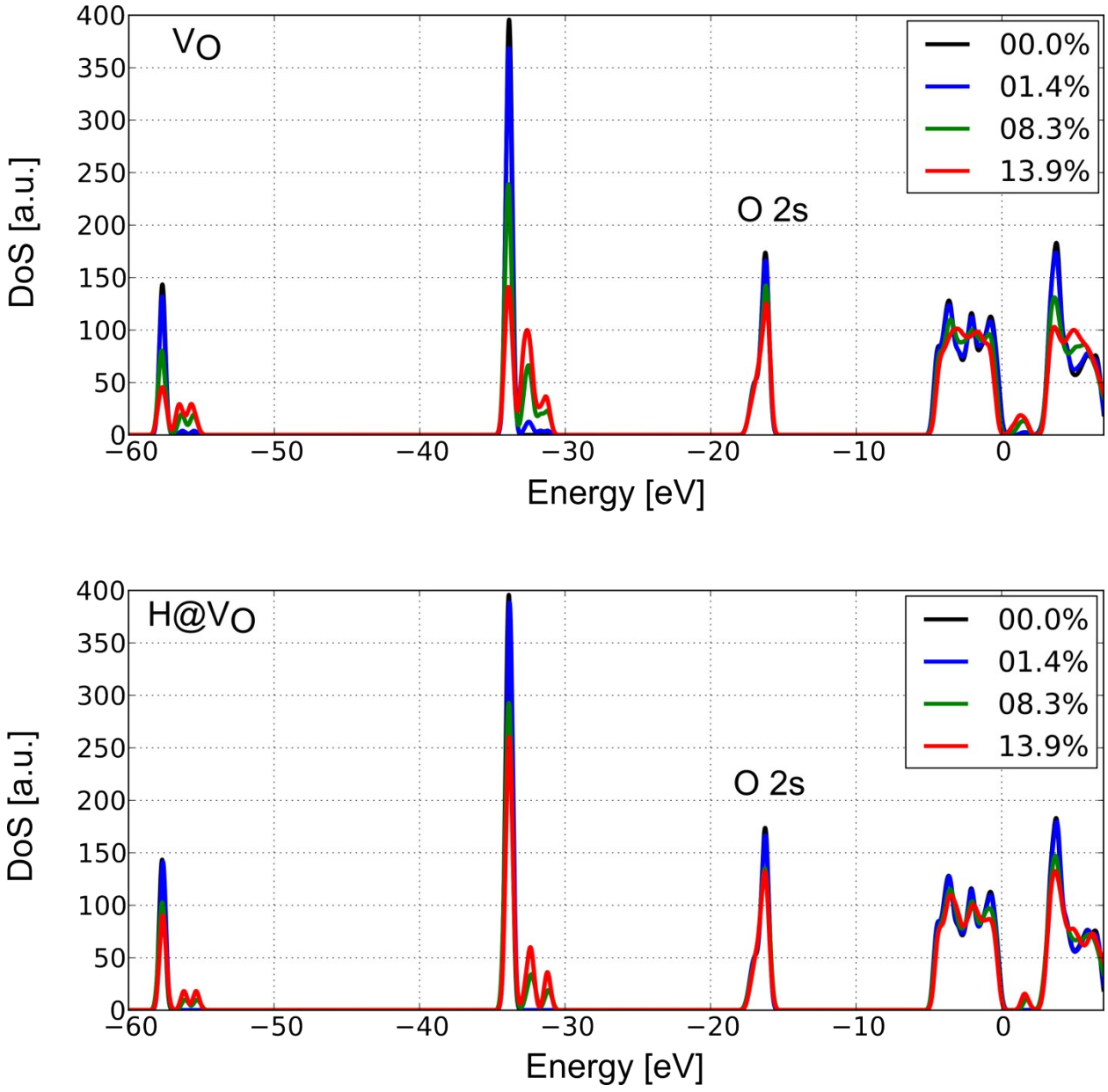

Fig. S2 Density of states (DoS) of anatase TiO_2 with different concentrations of oxygen vacancies V_O (top) and substitutional H_O defects (bottom) including the O 2s band. The latter is only weakly affected by the presence or absence of the considered defects. Therefore the center of the O 2s band was used to align the density of states plots in Fig. 9 and Fig. S1 for all defect concentrations. The highest occupied state of pristine TiO_2 was used to set the zero energy. Here, the results from the DFT+U calculations are shown.

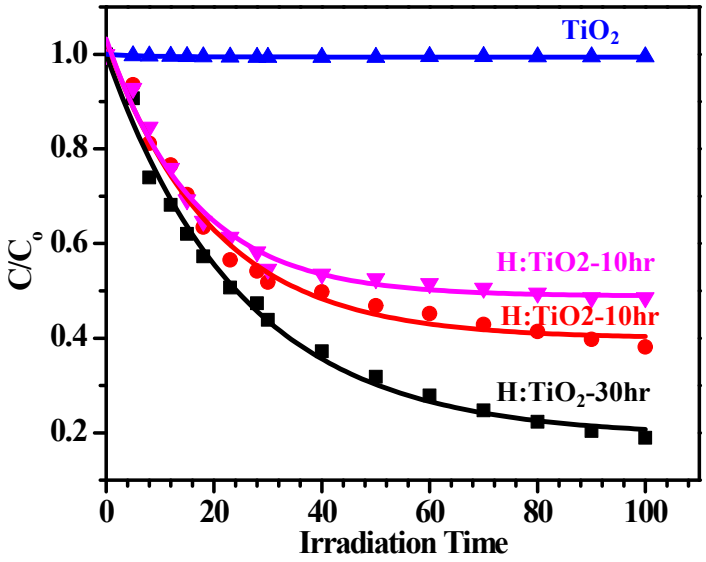

Fig. S3: Solar-light driven photocatalytic decomposition of phenol by different photocatalysts as a function of visible light irradiation time.

References

1. J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys., 2003, 118, 8207.
2. J. Paier, M. Marsman, K. Hummer, G. Kress, I. C. Gerber, and J. G. Angyan, J. Chem. Phys., 2006, 125, 249901.
3. J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys., 2006, 124, 219906.