

Supporting Information

Theoretical Insights into the Experimental Observation of Stable p-Type Conductivity and Ferromagnetic Ordering in Vacuum-Hydrogenated TiO₂

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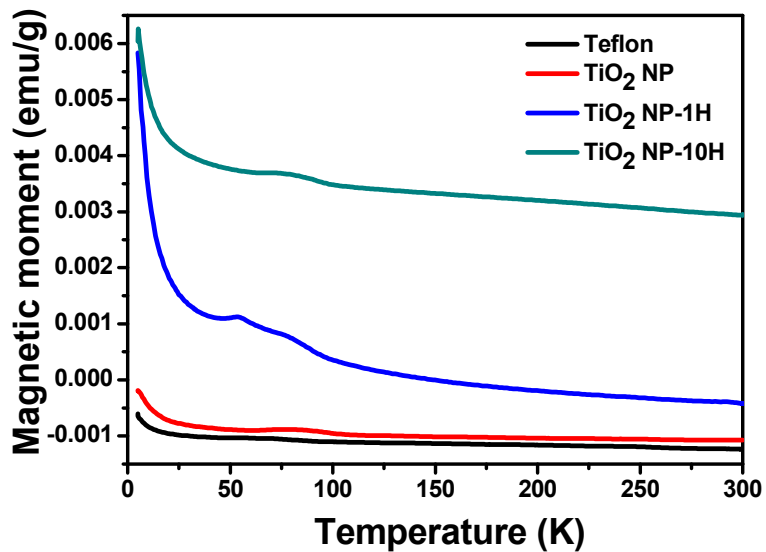


Figure S1. Field cooled M-T curves of Teflon, pristine TiO_2 and hydrogenated TiO_2 NPs at 5000 Oe illustrating increase in magnetization for hydrogen induced disordered TiO_2 NPs

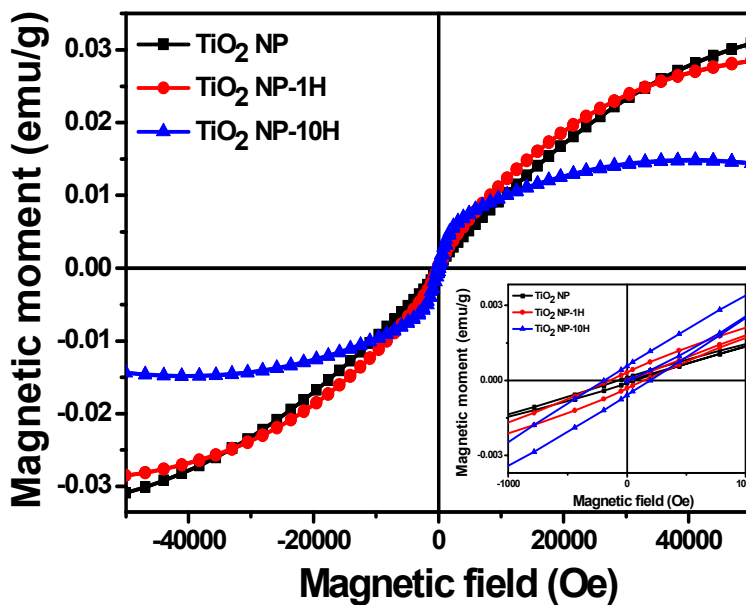


Figure S2. M-H curves of pristine and hydrogenated TiO_2 NPs at 5 K depicts the increase in magnetization at low temperature

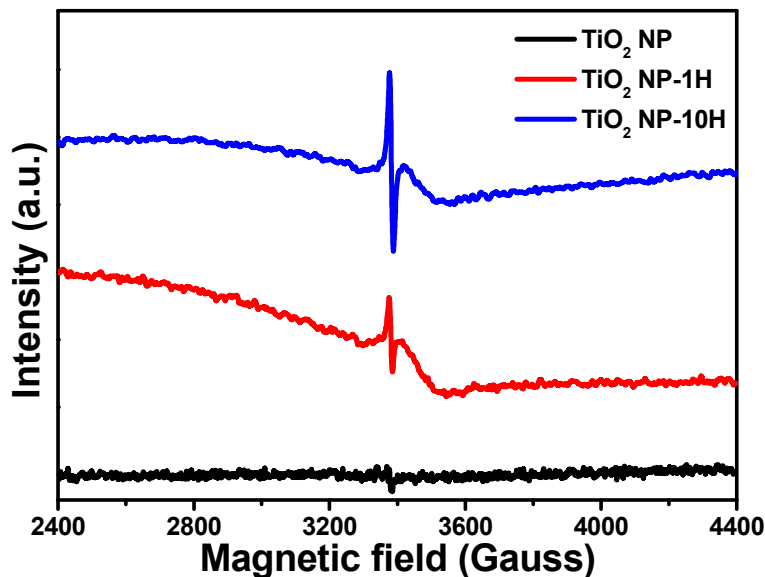


Figure S3. Room temperature EPR spectra of TiO_2 NP, TiO_2 NP-1H and TiO_2 NP-10H, discloses the unpaired electrons present in the hydrogenated TiO_2 NPs which significantly contributes for the ferromagnetic ordering

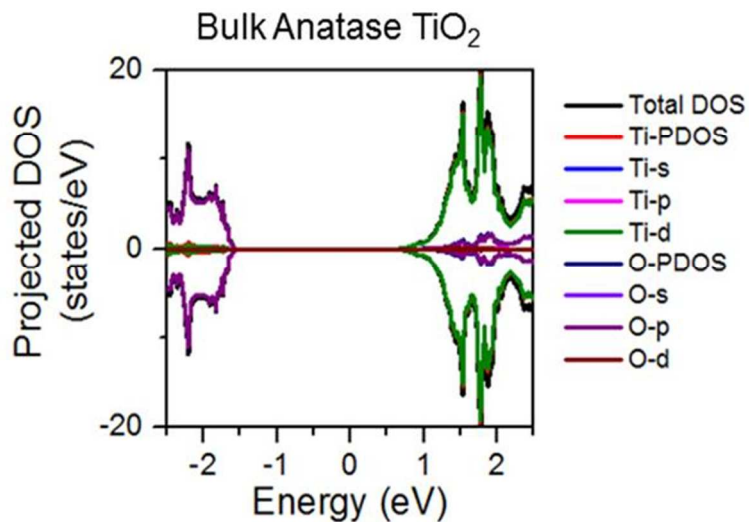


Figure S4. Bulk Anatase DOS, decomposed Projected DOS and different orbitals of Ti and O atoms. Valance band maximum is located at -1.6 eV

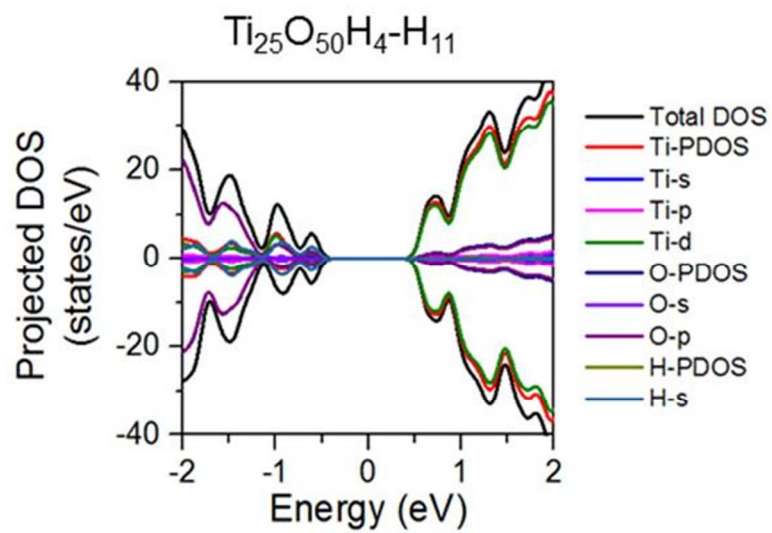


Figure S5. Hydrogenated $\text{Ti}_{25}\text{O}_{50}\text{H}_4\text{-H}_{11}$ nanocrystal DOS, decomposed Projected DOS and different orbitals of Ti, O, and H atoms.

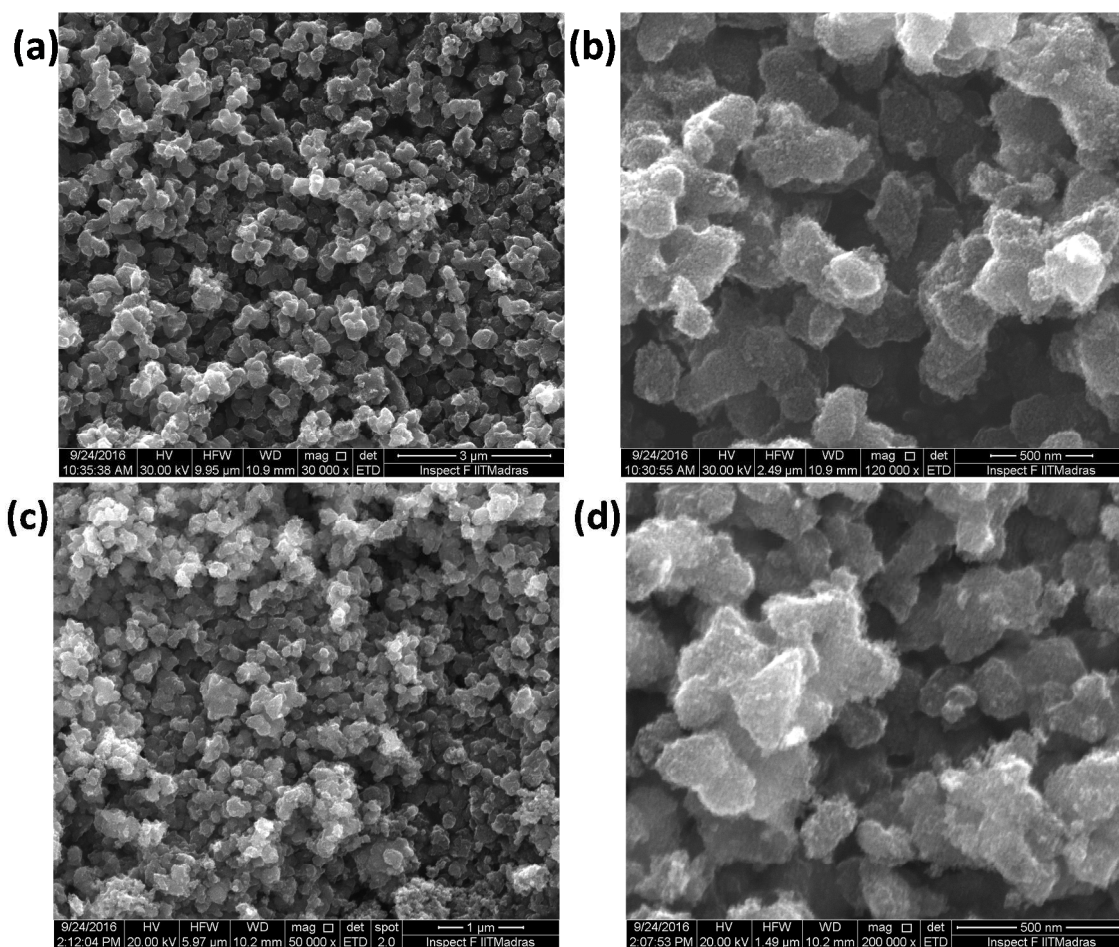


Figure S6. Field Emission Scanning Electron Microscopy images of hydrogenated (a and b) and pristine TiO₂ NPs (c and d)

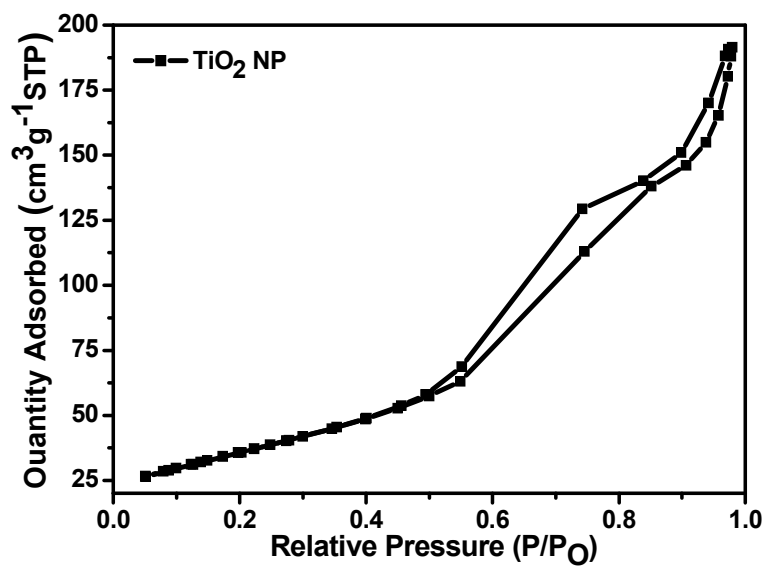


Figure S7. Nitrogen adsorption-desorption isotherms of pristine TiO₂ NPs, and the calculated BET surface area is 131.30 m²g⁻¹

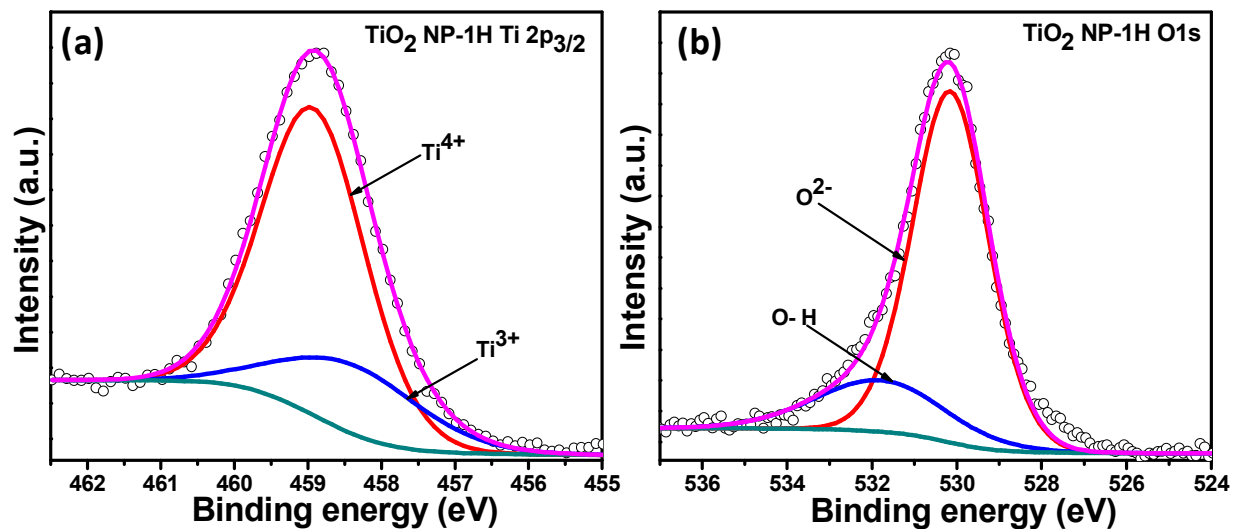


Figure S8. X-ray photoelectron spectra of (a) Ti 2p_{3/2} and (b) O 1s of TiO₂ NP-1H elucidates different doping in TiO₂ lattice after vacuum-hydrogenation

Table S1 Distribution of oxidation states and doping species obtained from XPS analysis

Peak	Position (eV)	% Conc.
Ti ⁴⁺	458.92	76.92
Ti ³⁺	458.37	23.08
O ²⁻	530.15	79.9
OH	531.8	20.01