Supplemental Information

Hydrogen Impurity Defects in Rutile TiO$_2$

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Fig. S1 Hall effect measurements of rutile TiO_2 single crystals at low temperatures. (a) Vacuum-annealed TiO_2, (b) gas-hydrogenated TiO_2, and (c) atom-hydrogenated TiO_2. The carrier concentration n, the resistivity ρ and the carrier mobility μ were obtained through linear fitting between the measured Hall resistance and the applied magnetic field.
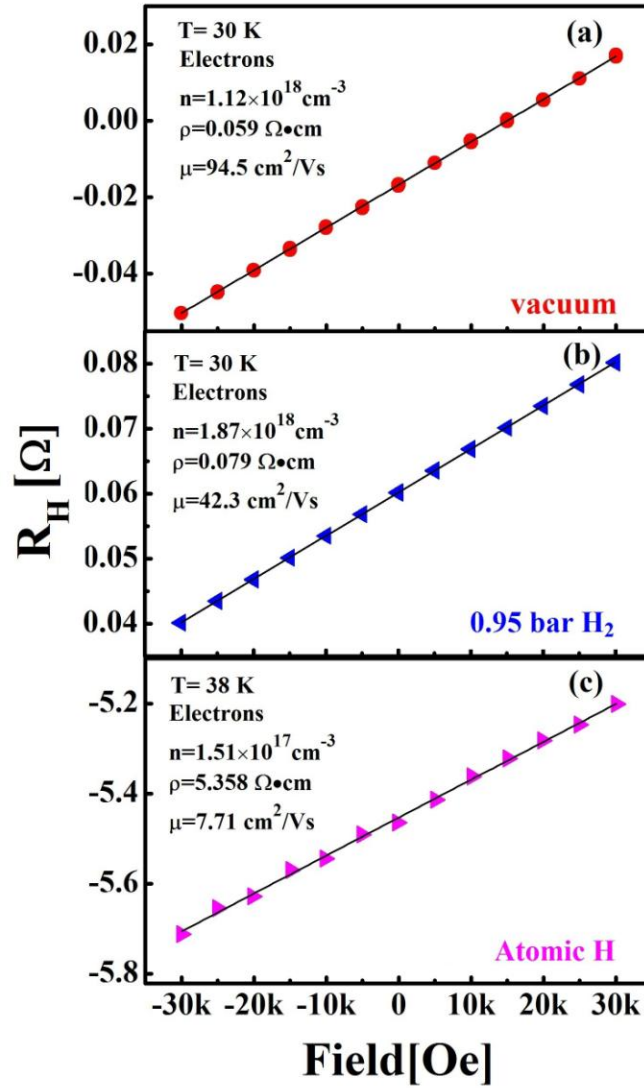
Fig. S2 XRD patterns of rutile TiO_2 samples. The TiO_2 single crystals were ground into powders for the XRD measurements.
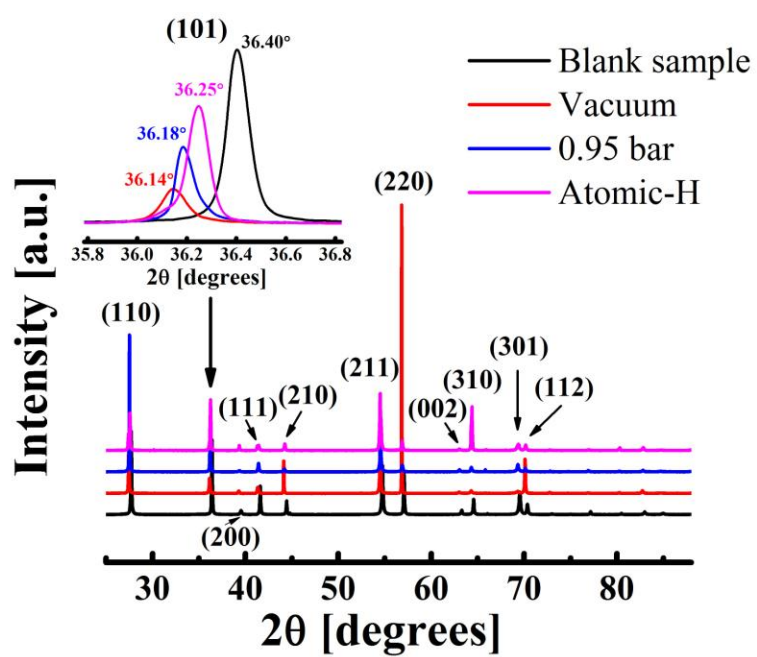
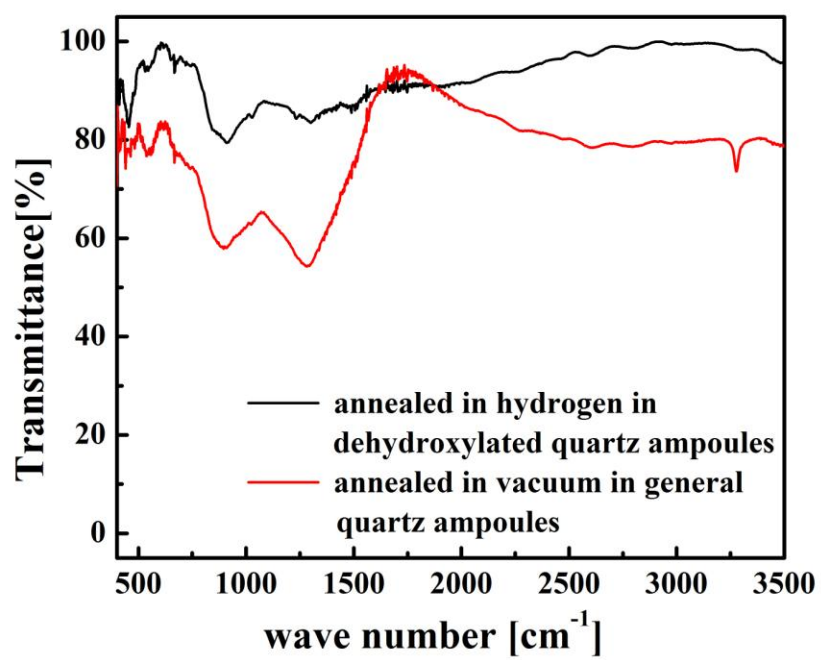Fig. S3 Infrared absorption spectra of annealed TiO$_2$.

Table I Bader analyses.

Atom	Bader charge	Distance	Atom	Bader charge	Distance
Blank sample			O$_4$	7.0288	0.8484
O	6.9767	0.844	Ti$_1$	2.0386	0.8313
Ti	2.0453	0.886	Ti$_2$	2.0316	0.8761
Vo			Ti$_3$	2.0390	0.8326
O$_1$	7.0156	0.8447	Ti$_4$	2.0317	0.8705
O$_2$	7.0156	0.8774	**Ho**		
O$_3$	7.0156	0.8405	H	1.5039	0.7438
Ti$_1$	2.0953	0.8041	O$_1$	6.9946	0.8447
Ti$_2$	2.0953	0.8041	O$_2$	6.9946	0.8447
Ti$_3$	2.0987	0.8128	O$_3$	6.9874	0.8412
Hi			O$_4$	6.9875	0.8412
H	0.3565	0.0704	Ti$_1$	2.0788	0.8322
O$_1$	6.9981	0.8248	Ti$_2$	2.0787	0.8312
O$_2$	7.1875	0.7024	Ti$_3$	2.0925	0.8601
O$_3$	7.0013	0.8284			