**Supplementary Information**

**Introducing oxygen vacancies in TiO2 lattice through trivalent iron to enhance the photocatalytic removal of indoor NO**

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**Table S1.** The peak value and the crystal plane spacing of (101) peak for all samples

|  |  |  |
| --- | --- | --- |
| Sample | Peak value, 2*θ* / (°) | Crystal plane spacing / Å |
| TiO2 | 25.362 | 3.5089 |
| 1%Fe–TiO2 | 25.359 | 3.5093 |
| 2%Fe–TiO2 | 25.344 | 3.5113 |
| 3%Fe–TiO2 | 25.287 | 3.5191 |

**Table S2.** The specific surface area, pore volume and pore size of the samples

|  |  |  |  |
| --- | --- | --- | --- |
| Sample | Specific surface area / (m2/g) | Pore volume / (cm3/g) | Pore diameter / nm |
| TiO2 | 116.25 | 0.24 | 7.56 |
| 1%Fe-TiO2 | 111.11 | 0.24 | 7.84 |
| 2%Fe-TiO2 | 120.20 | 0.25 | 7.45 |
| 3%Fe-TiO2 | 111.97 | 0.24 | 7.66 |

**Table S3.**  The elemental composition of as-prepared samples (molar ratio)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Ti / % | O / % | Fe / % | Fe:Ti / % | OA:OL / % |
| TiO2 | 31.51 | 68.49 | - | - | 12.5 |
| 1%Fe–TiO2 | 28.98 | 70.80 | 0.22 | 0.76 | 24.4 |
| 2%Fe–TiO2 | 29.09 | 70.34 | 0.57 | 1.96 | 31.8 |
| 3%Fe–TiO2 | 29.11 | 70.10 | 0.78 | 2.68 | 24.8 |

**Table S4.**  The comparison of NO removal ability for different photocatalysts under visible light irradiation

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Photocatalysts | Photocatalytic experimental conditions | Photocatalytic activities | | |
| *η*1a | *η*2b | Pc |
| OVs-TiO2[1] | Xe lamp of 300W, *λ*>400 nm  *c*0=600 ppb  *T*=298 K  flow rate=1 L/min | 48% | 63% d | 131% |
| C-TiO2[2] | Mercury lamp of 450 W, *λ*>400 nm  *c*0=1 ppm  *T*=298 K  flow rate=100 mL/min | - | 29% | - |
| OVs-TiO2[3] | Mercury lamp of 450 W, *λ*>400 nm  *c*0=1 ppm  *T*=298 K  flow rate=100 mL/min | 22% | 45% | 204% |
| Ag/TiO2[4] | Xe lamp of 300 W, *λ*>420 nm  *c*0=600 ppb | 22% | 63% | 286% |
| C3N4/Ti3+-TiO2[5] | Xe lamp of 300 W, *λ*>420 nm  *c*0=400 ppb  flow rate=1.2 mL/min | 13.4% | 25% | 186% |
| Bi4O5Br2/TiO2[6] | Xe lamp of 300 W  *c*0=430 ppb  RH=30±5% | 23.53% | 54.33% | 230% |
| C3N4[7] | Mercury lamp of 450 W, *λ*>400 nm  *c*0=1 ppm  flow rate=100 mL/min | - | 32.5% | - |
| Bi2WO6/BiOCl[8] | Xe lamp of 300 W, *λ*>420 nm  *c*0=100 ppm | - | 26% | - |
| This work | Mercury lamp of 450 W, *λ*>400 nm  *c*0=1 ppm  *T*=298 K  flow rate=100 mL/min | 9% | 36% | 400% |

a Removal ratio of NO before modification

b Removal ratio of NO before modification

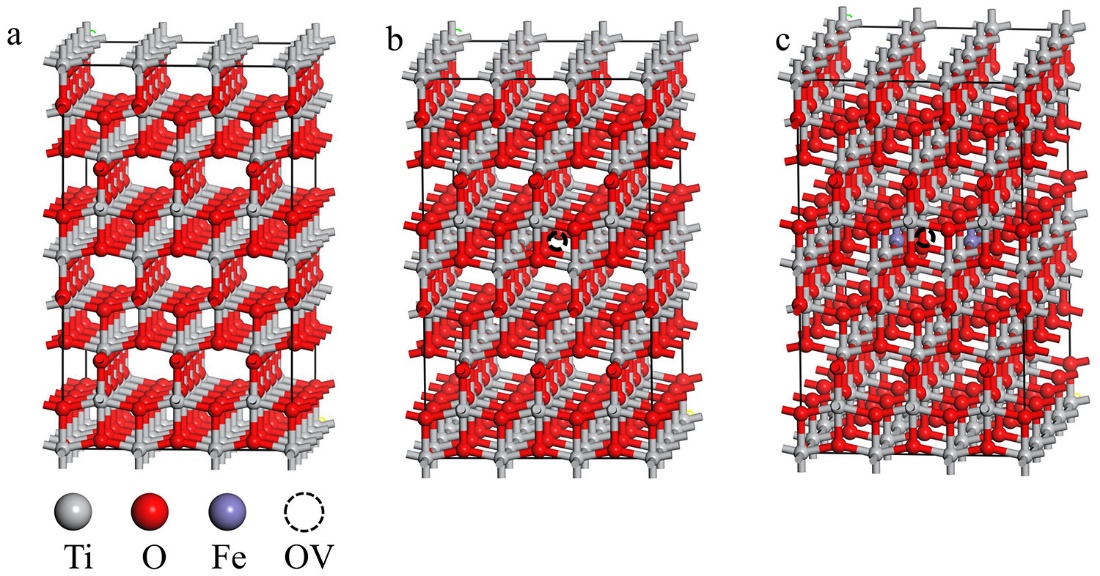
c (*η*2-*η*1)/ *η*1×100%

**Table S5.** TPRL parameters of TiO2 and Fe-TiO2 photocatalysts

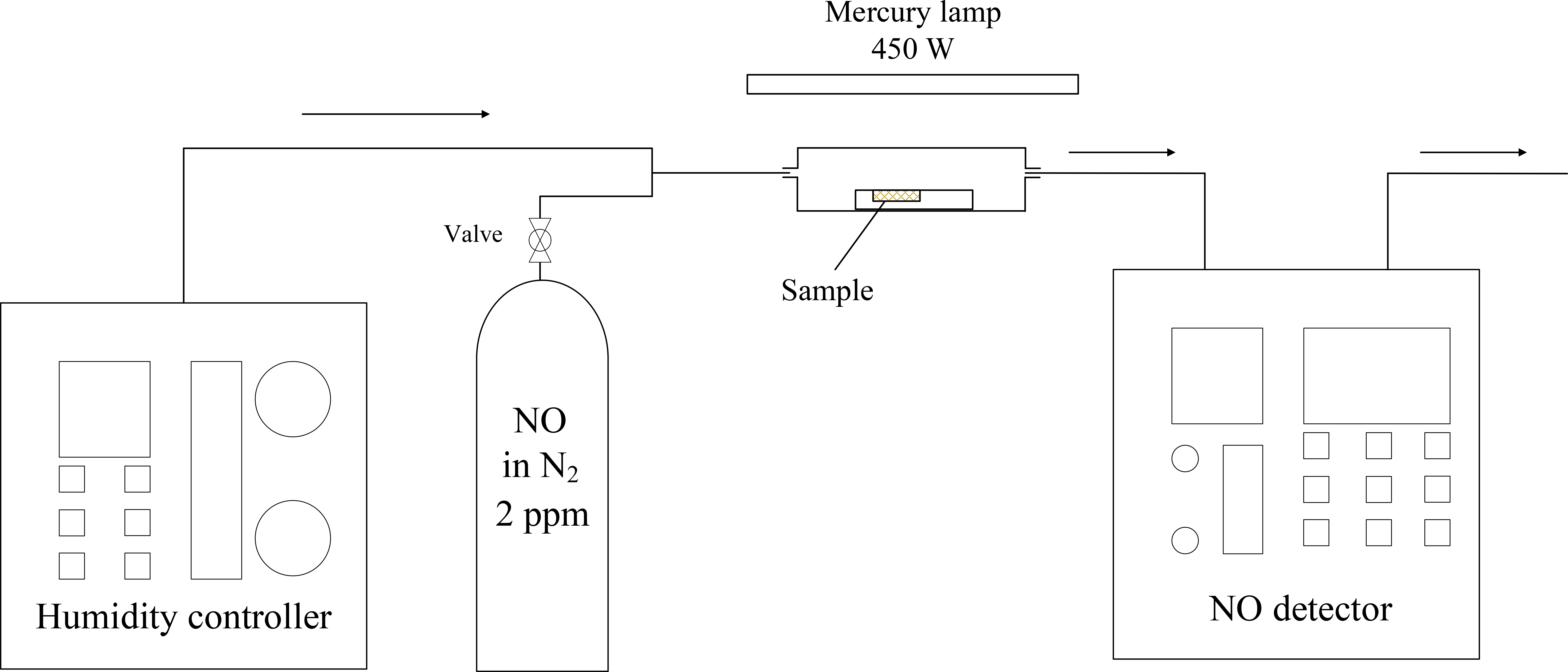
|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | *τ*1 / ns | Error of *τ*1 / ns | *f*1 / % | *τ*2 / ns | Error of *τ*2 / ns | *f*2 / % | *τ*ave / ns |
| TiO2 | 1.125 | 1.202×10-2 | 55.96 | 5.880 | 1.107×10-1 | 44.04 | 3.22 |
| 1%Fe–TiO2 | 1.125 | 1.445×10-2 | 41.73 | 6.075 | 7.527×10-2 | 58.27 | 4.00 |
| 2%Fe–TiO2 | 1.099 | 1.455×10-2 | 40.55 | 6.150 | 7.680×10-2 | 59.45 | 4.10 |
| 3%Fe–TiO2 | 1.176 | 1.237×10-2 | 56.39 | 6.136 | 1.082×10-1 | 43.61 | 3.34 |

**Table S6.** The calculated effective masses of electrons and holes in different directions in the reciprocal space of TiO2 and Fe-TiO2 (*m*0 was defined as the mass of free electrons)

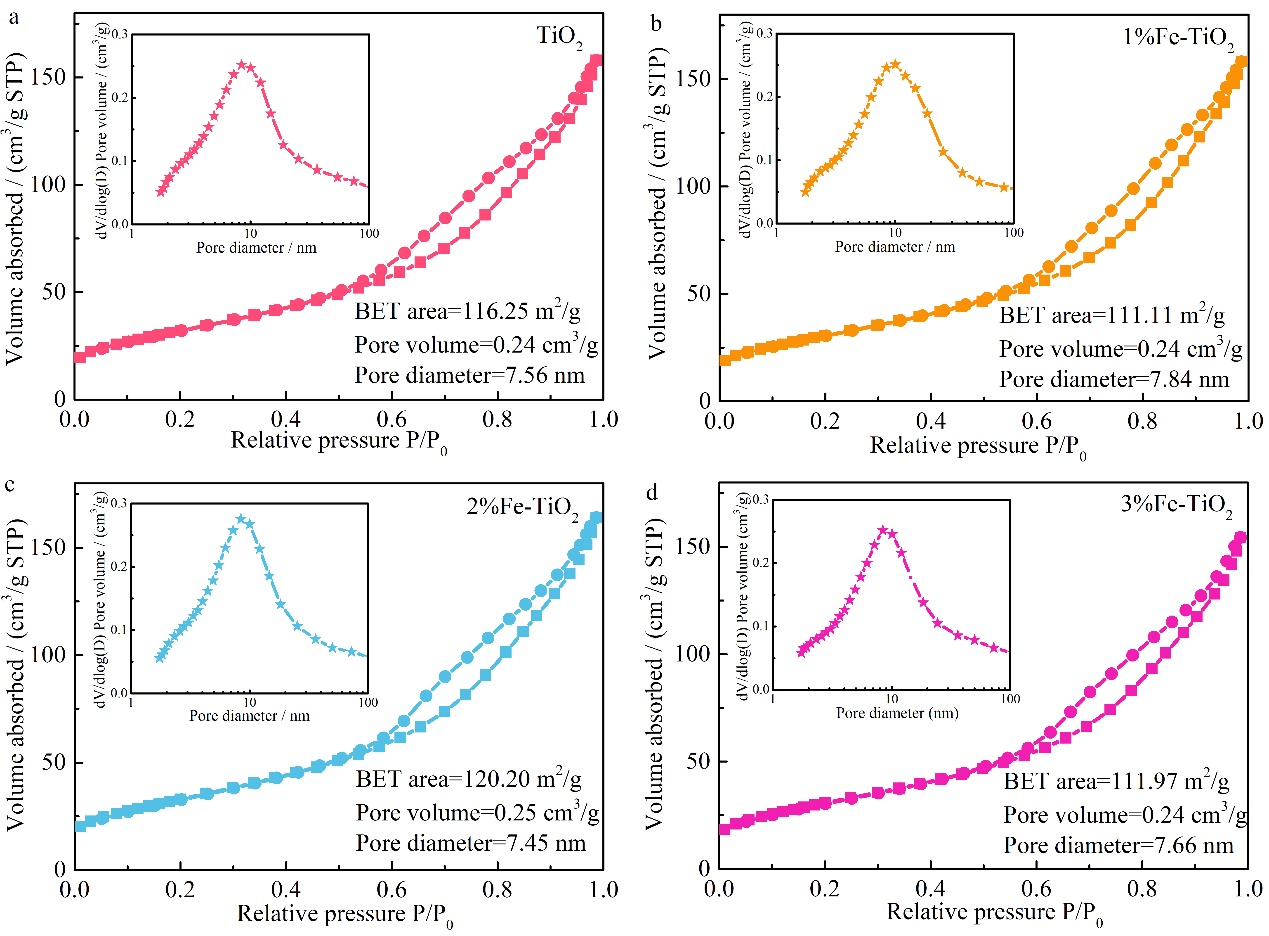
|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Direction | *m*e\*/*m*0 | *m*h\*/*m*0 | *D* |
| TiO2(up/down) | G→F | 0.86 | 3.16 |  |
|  | G→Z | 7.26 | 2.28 |  |
| average |  | 4.06 | 2.72 | 1.49 |
| Fe-TiO2 (up) | G→F | 0.88 | 28.34 |  |
|  | G→Z | 27.87 | 75.32 |  |
| average |  | 14.38 | 51.83 | 3.61 |
| Fe-TiO2 (down) | F→G  (F→Q) | 7.48 | 1.78 |  |
| average |  | 7.48 | 1.78 | 4.20 |



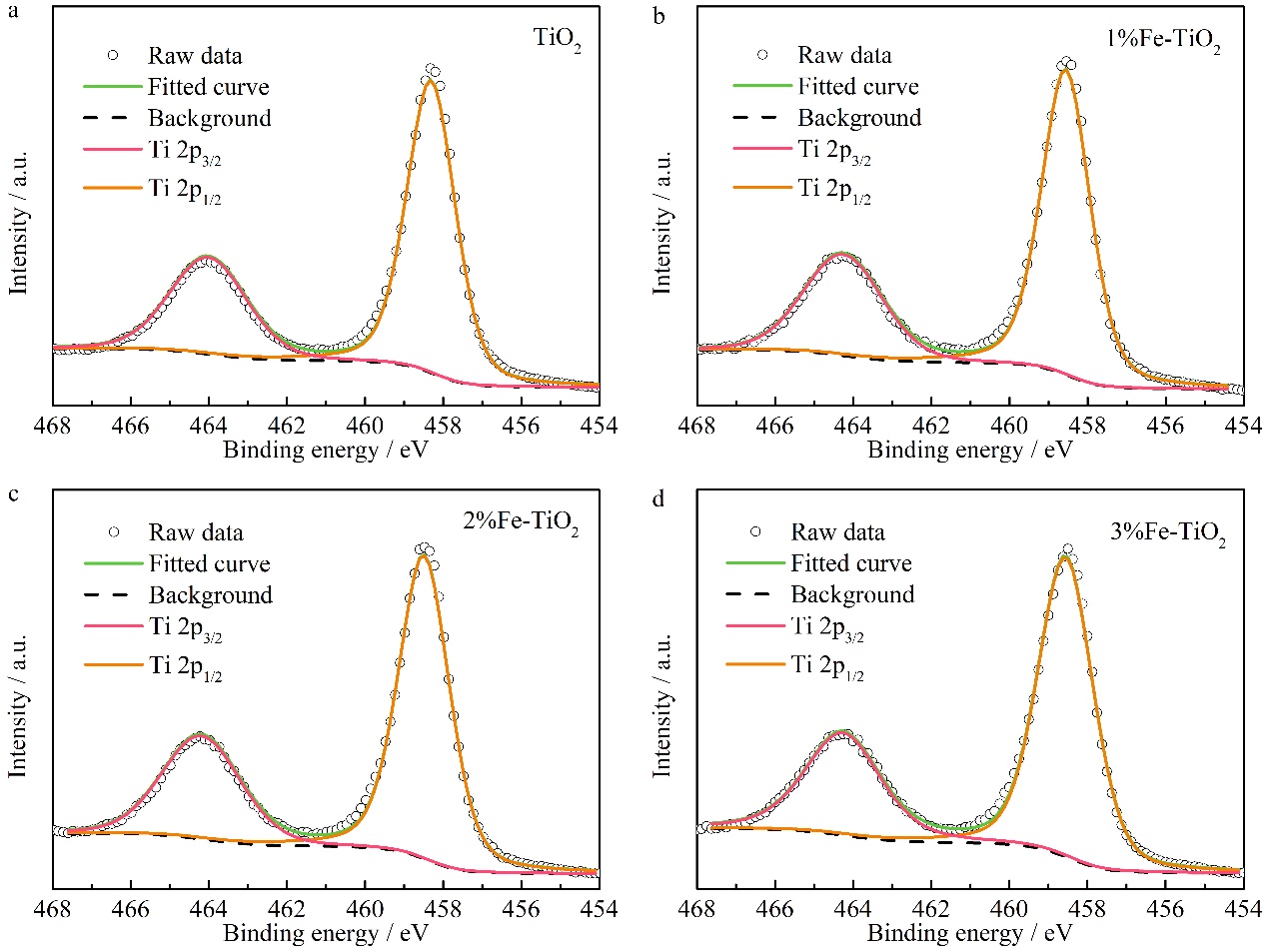
**Fig. S1.**  The structure models of (a) TiO2(Ti96O192), (b) OVs-TiO2(Ti96O191), and (c) Fe–TiO2(Ti94Fe2O191).



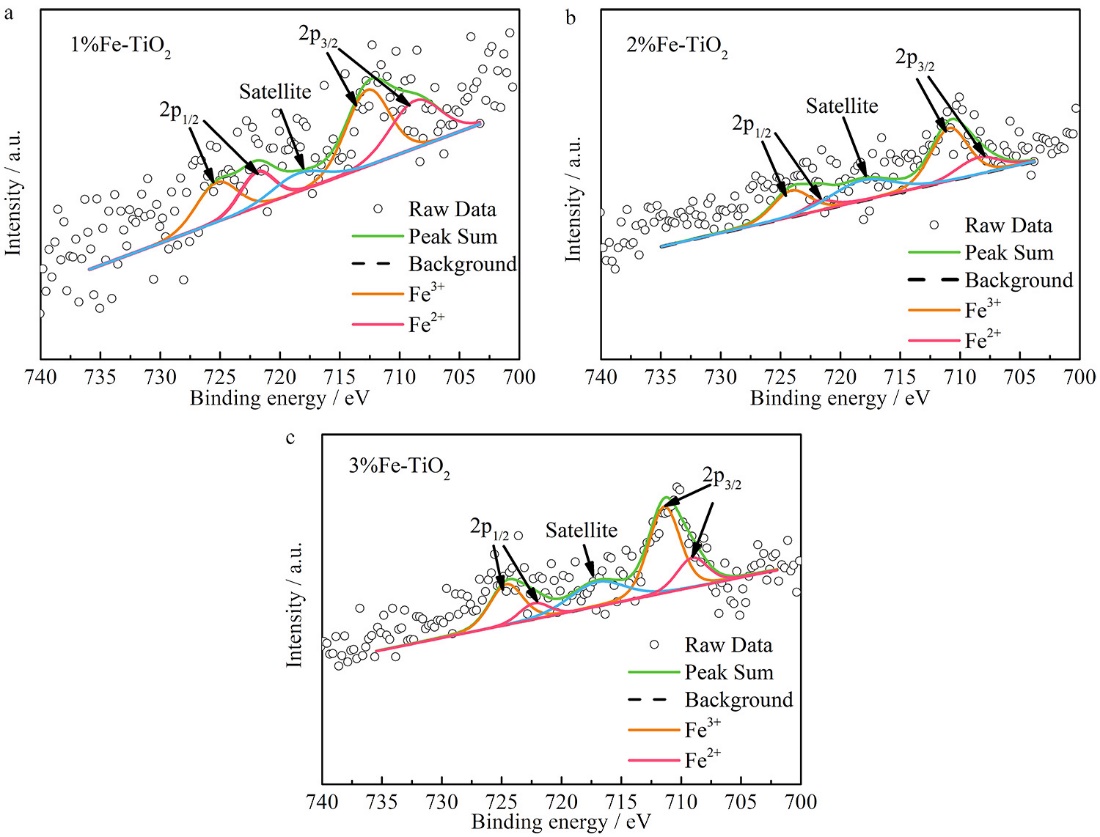
**Fig. S2.**  The schematic illustration of NO photocatalytic removal system.



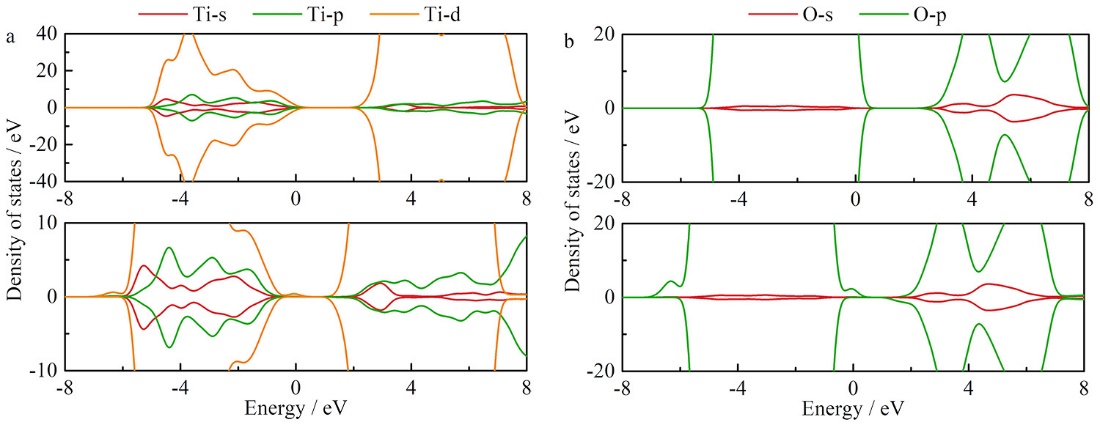
**Fig. S3.**  The nitrogen gas adsorption isotherms of (a) TiO2, (b) 1%Fe–TiO2, (c) 2%Fe–TiO2, and (d) 3%Fe–TiO2.



**Fig. S4.** Detailed analysis of Ti 2p peaks for (a) TiO2, (b) 1%Fe–TiO2, (c) 2%Fe–TiO2 and (d) 3%Fe–TiO2.



**Fig. S5.** Detailed analysis of Fe 2p peaks for (a) 1%Fe-TiO2, (b) 2%Fe-TiO2 and (c) 3%Fe-TiO2.



**Fig. S6.**  (a) Ti states and (b) O states of TiO2 and Fe–TiO2.

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