Supplementary Information

Rhodium Doping Augments Photocatalytic Activity of Barium Titanate: Effect of Electronic Structure Engineering

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**Figure S1.** pdos of 2 x 2 x 2 supercell of Rh doped BaTiO$_3$ (case A) with one Rh in Ti site (lavender) indicated as Rh* and another Rh in Ba site (pink).
Figure S2. Electronic structure and DOS of 2 x 2 x 2 supercell of Rh doped BaTiO$_3$ with two Rh in Ba sites.
**Figure S3.** XRD patterns of synthesized samples showing (110) peak shift to higher θ values.
Figure S4. XPS survey spectrum of 0.5 Rh.
Figure S5. Spot EDX of a) Ba, b) Ti, c) O and d) Rh in 0.5 Rh.
Figure S6. BET surface area analysis of BaTiO$_3$ (inset shows pore size distribution).
Figure S7. a) XRD of 0.9 Rh, b) UV and c) PL spectra of BaTiO$_3$ and 0.9 Rh and d) photocatalytic degradation of MB using 0.9 Rh.
Figure S8. Cyclic stability test of 0.5 Rh.
Table S1. Comparison of photocatalytic activity of 0.5 Rh sample with reported literatures.

| Photocatalysts                        | Light source                                                                 | Pollutant used       | Degradation extent and Time | Reference                                      |
|---------------------------------------|-------------------------------------------------------------------------------|----------------------|-----------------------------|------------------------------------------------|
| Rh doped BaTiO₃                       | Visible light source (High pressure 250 W Hg vapor lamp)                     | Methylene Blue       | 96 %, 120 min               | Present work                                   |
| N doped BaTiO₃                        | Visible light source (300 W Xe lamp, UV cutoff filter)                       | Rhodamine B          | 50 %, 240 min               | Cao et al. 2014 [1]                            |
| BaTiO₃@g-C₃N₄ composite               | Solar simulator (200 W Xe lamp)                                              | Methyl orange        | 76 %, 360 min               | Xian et al. 2015 [2]                           |
| BaTiO₃@graphene nanocomposite         | Visible light source (500 W Xe lamp, UV cutoff filter)                       | Methylene blue       | 69.5 %, 480 min             | Wang et al. 2015 [3]                           |
| Mn doped BaTiO₃                       | Visible light source (300 W Tungsten lamp)                                  | Methylene blue       | 97.04 %, 360 min            | Nageri and Kumar 2018 [4]                      |
| Auₓ/BaTiO₃ heterostructure            | All spectrum light source (300 W Xe lamp, cutoff filter)                    | Methyl orange        | 80 %, 75 min, 97 %, 75 min  | Xu et al. 2019 [5]                             |
| W doped BaTiO₃                        | 18 UV lamps as UV light source and 2 metal halide lamps as visible light source | Tetracycline         | UV-A light: 77 % visible light: 80 % in 180 min | Demircivi and Simsek 2019 [6]                  |
| Fe-Cr co-doped BaTiO₃                | Solar simulator (Xe lamp)                                                    | Methyl orange        | 94 %, 90 min                | Amaechi et al. 2019 [7]                        |
| Ce doped BaTiO₃                       | UV light source (254 nm) and visible light source (400–750 nm, 300 W tungsten-halogen lamp) | Methylene blue, Methyl violet, Congo red | 90.2 %, 120 min, 82.4 %, 120 min, 78.5 %, 120 min | Senthilkumar et al. 2019 [8]                    |
| Cr³⁺ doped BaTiO₃                     | Solar simulator (150 W Xe lamp)                                              | Methyl orange        | 87 %, 90 min                | Amaechi et al. 2019 [9]                        |
| Ag doped BaTiO₃ composite             | UV-vis light source (300 W Xe lamp)                                          | Rhodamine B          | 61 %, 75 min, 83 %, 75 min  | Xu et al. 2019 [10]                            |
| BaTiO₃@graphene oxide composite       | UV-vis light source (Xe lamp)                                                | Methylene blue       | 95 %, 180 min               | Mengting et al. 2019 [11]                      |
| Fe doped BaTiO₃                       | Solar simulator (150 W Xe lamp)                                              | Methyl orange        | 75 %, 90 min                | Amaechi et al. 2019 [12]                       |
| BaTiO₃@carbon                         | 18 UV lamps as Tetracycline                                                  | UV-A light: 96 %     |                             | Demircivi et                                   |
| Fiber Catalyst                        | UV-A light source and 2 metal halide lamps as visible light source | % Visible light: 92% in 180 min | Xiao et al. 2020 [14] |
|--------------------------------------|-------------------------------------------------------------------|---------------------------------|------------------------|
| N-Ni co-doped (Na_{0.5}Bi_{0.5})TiO_{3}-BaTiO_{3} | 300 W Xe lamp (PLS-SXE300+/UV)                                   | Rhodamine B Dibenzothiophene 92.4%, 80 min 90.37%, 150 min |                       |
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