

Supporting Information

Electronic and photocatalytic properties of N/F co-doped anatase TiO₂

Yafei Zhao^a, Wei Wang^a, Can Li^b and Liang He^{*a}

^aNational Laboratory of Solid State Microstructures, School of Electronic Science and Engineering and Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China

^bCenter for Coordination Bond Engineering, College of Materials Science and Engineering, China Jiliang University, Hangzhou 310018, China

Corresponding Authors

* L.H: heliang@nju.edu.cn

SUPPORTING INFORMATION

S1. All possible configurations

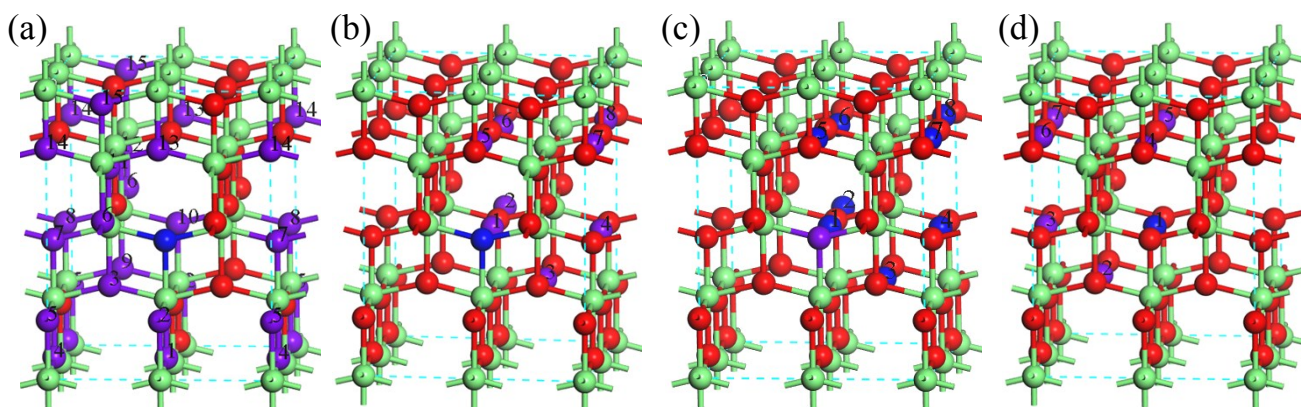


Figure S1. (Color online) The crystal structures of four different cases: (a) N_s-F_s co-doped TiO₂, (b) N_s-F_i co-doped TiO₂, (c) N_i-F_s co-doped TiO₂ and (d) N_i-F_i co-doped TiO₂, where green, red, blue and purple balls are the Ti, O, N and F atoms, respectively. The number denotes the different substituted positions of N or F atoms.