C, N, S, and F-doped anatase TiO$_2$ (101) with oxygen vacancies: Photocatalysts active in the visible region

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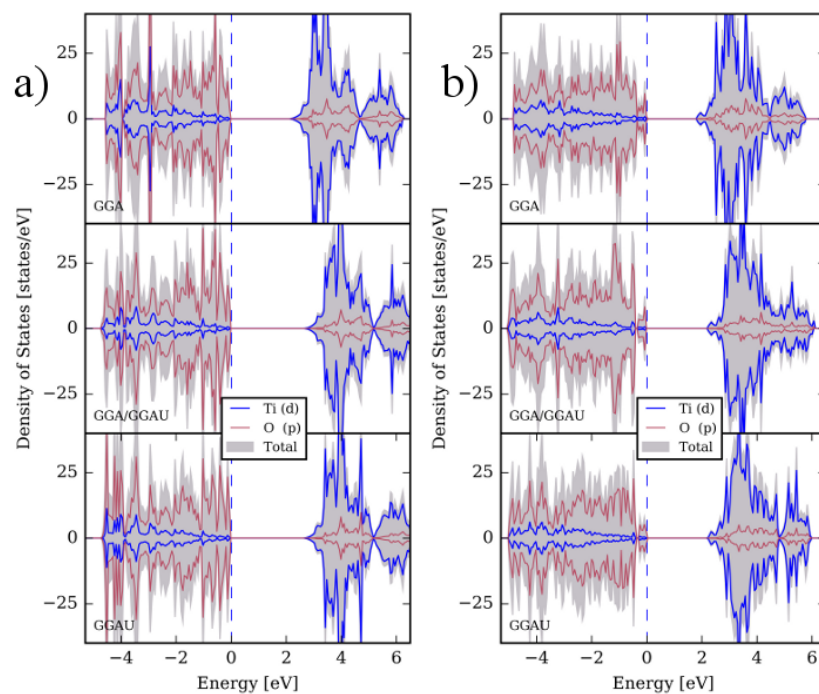
Supplementary Materials

Figure S1. The total and partial density of states of the three relaxation methodologies for anatase TiO$_2$. a) The bulk supercell; b) The TiO$_2$ (101) surface. The Fermi level corresponds to the zero energy.
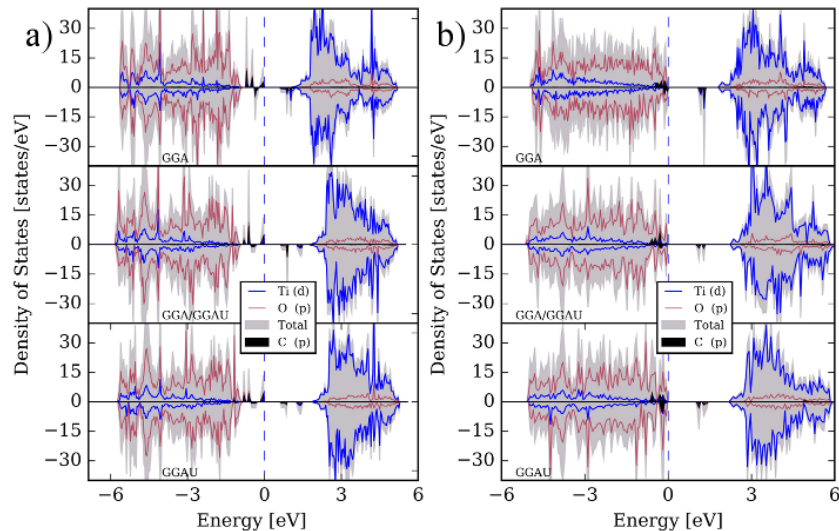
Figure S2. The total and partial density of states of the three relaxation methodologies for C-doped anatase TiO_2. a) The bulk supercell; b) The TiO_2 (101) surface.
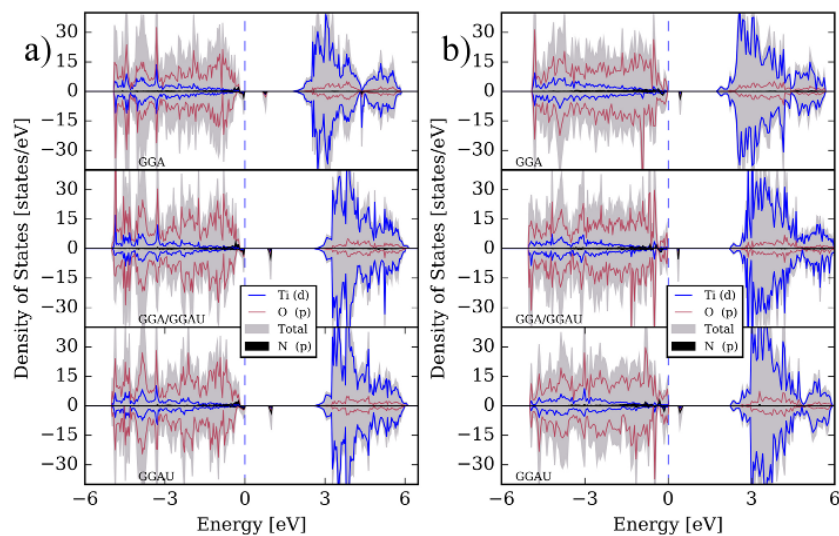

Figure S3. The total and partial density of states of the three relaxation methodologies for N-doped anatase TiO_2. a) The bulk supercell; b) The TiO_2 (101) surface.
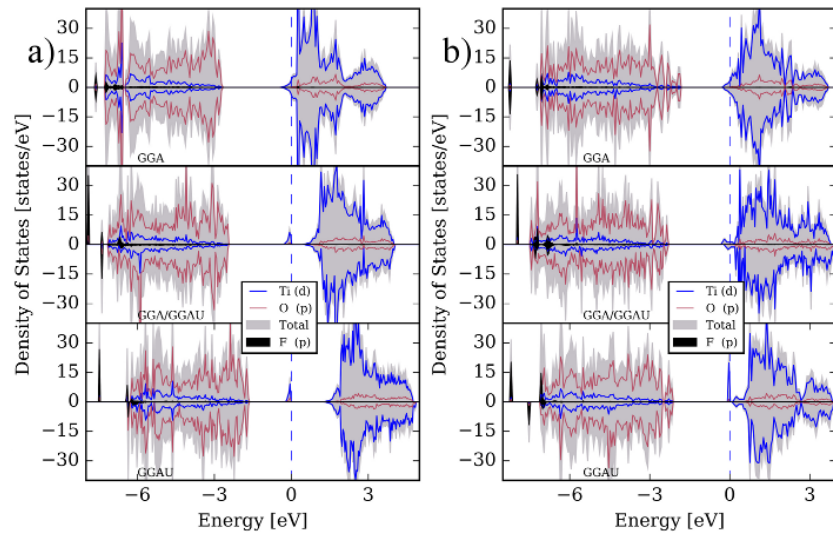
Figure S4. The total and partial density of states of the three relaxation methodologies for F-doped anatase TiO_2. a) The bulk supercell; b) The TiO_2 (101).
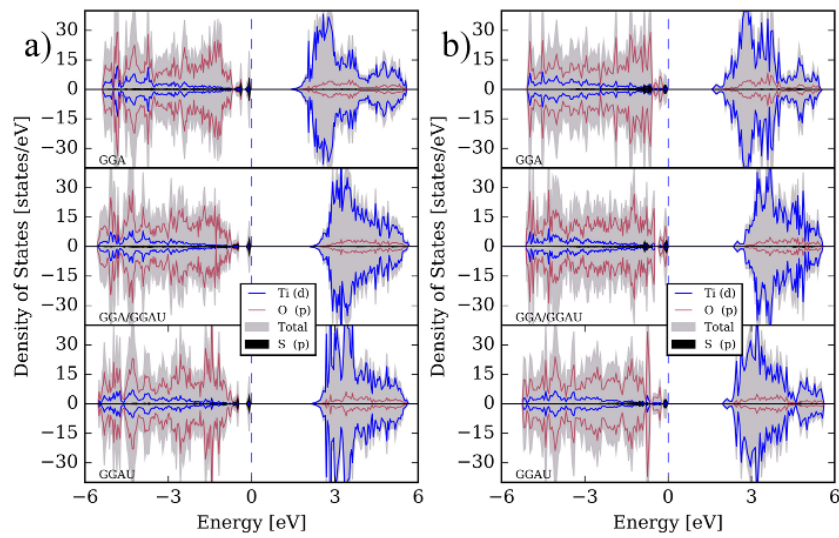

Figure S5. The total and partial density of states of the three relaxation methodologies for S-doped anatase TiO_2. a) The bulk supercell; b) The TiO_2 (101) surface.