**Supporting Information：**

# Theoretical study on catalytic degradation of sulfacetamide on anatase $TiO_2$ (001) and (101) surface

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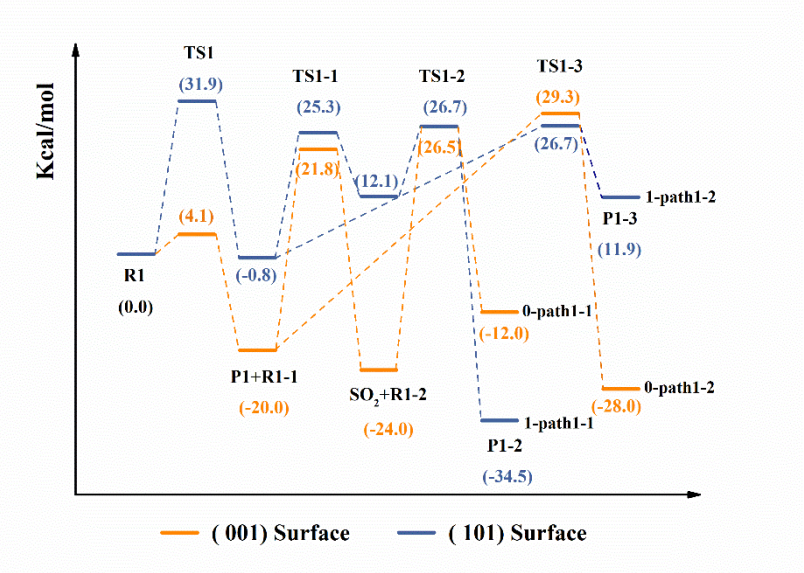
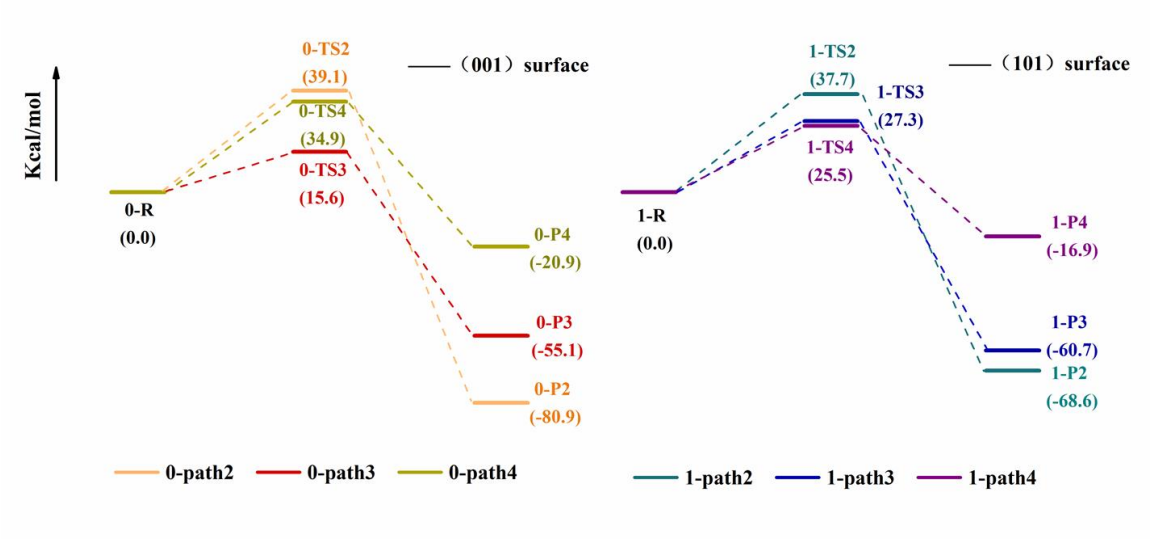



**Figure S1.** Energy barrier diagrams of (001) and (101) surface path1 in vacuum calculated using PBE+U+D3 method.

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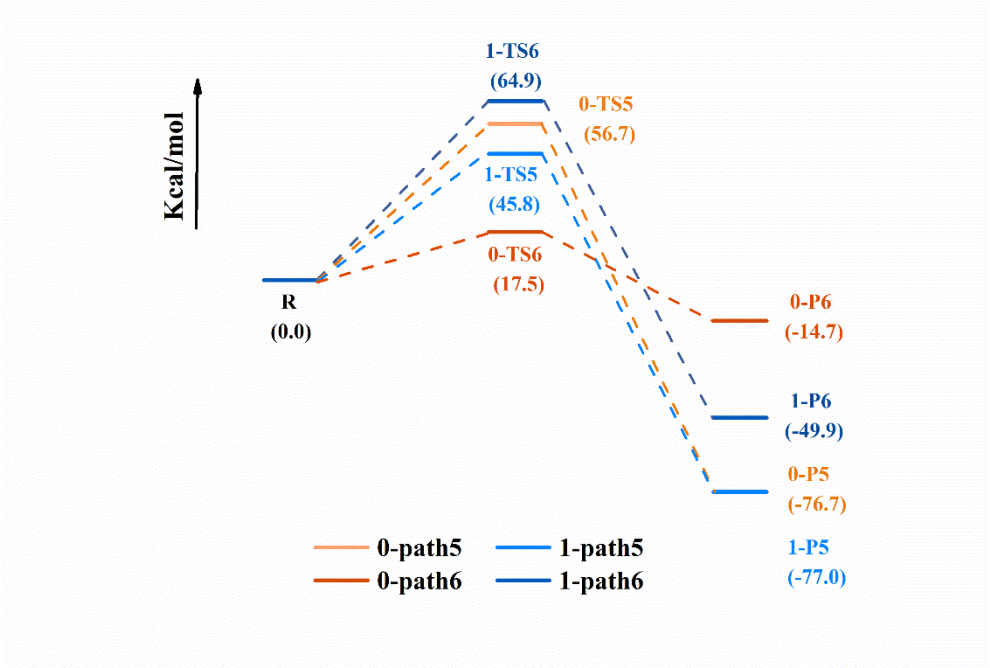



**Figure S3.** Energy barrier diagrams of (001) and (101) surface path5~6 in vacuum calculated using PBE+U+D3 method.

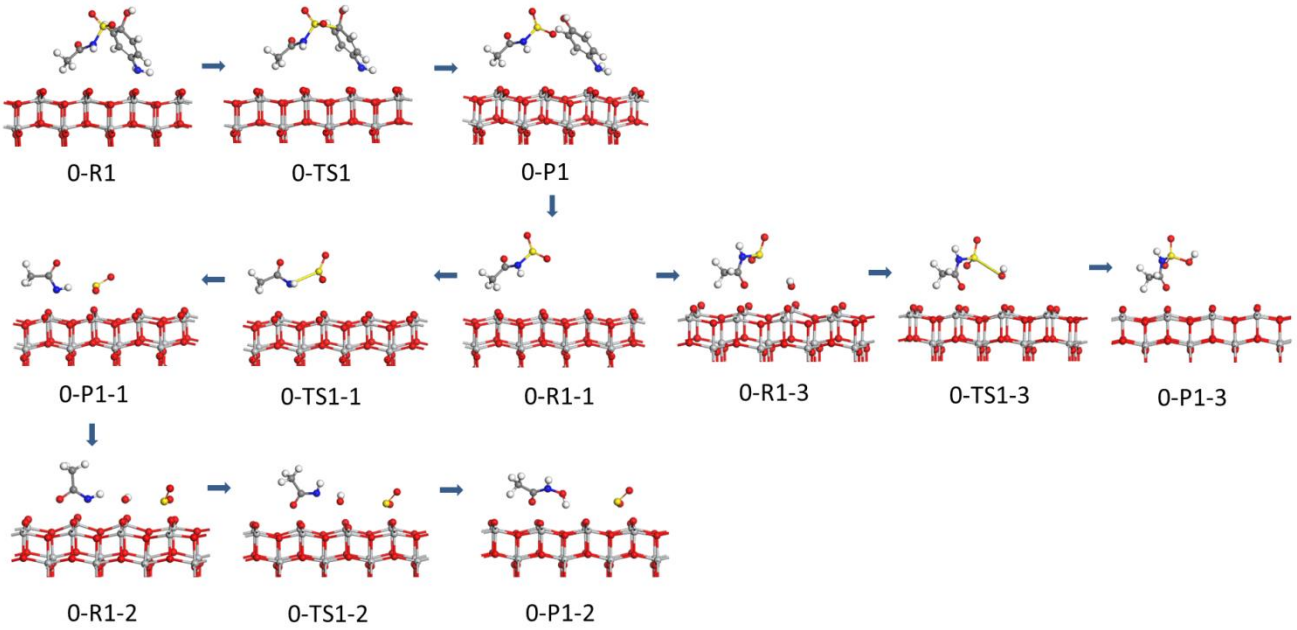
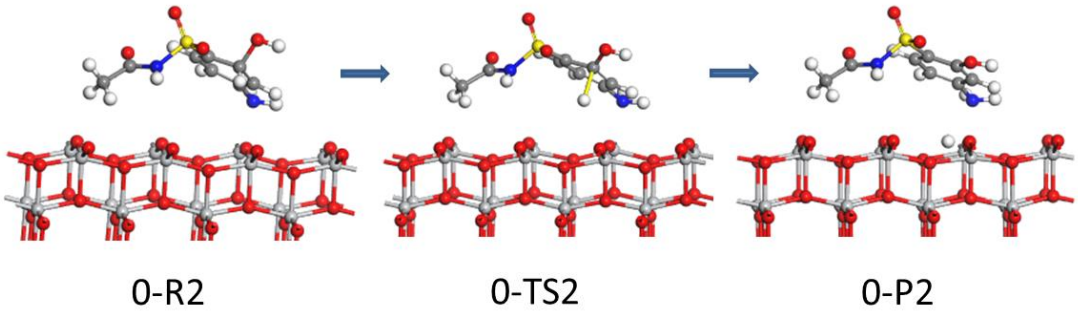



**Figure S4.** The configuration of reactants, transition states and products involved in the path1 process on （001）surface.

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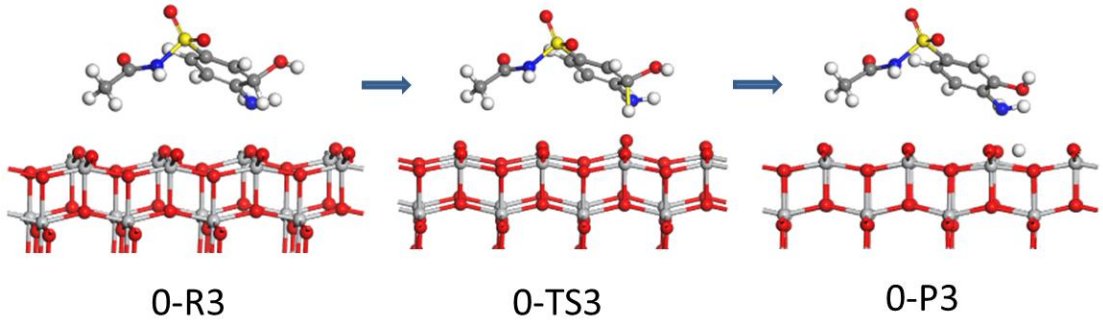



**Figure S6.** The configuration of reactants, transition states and products involved in the path3 process on （001）surface.

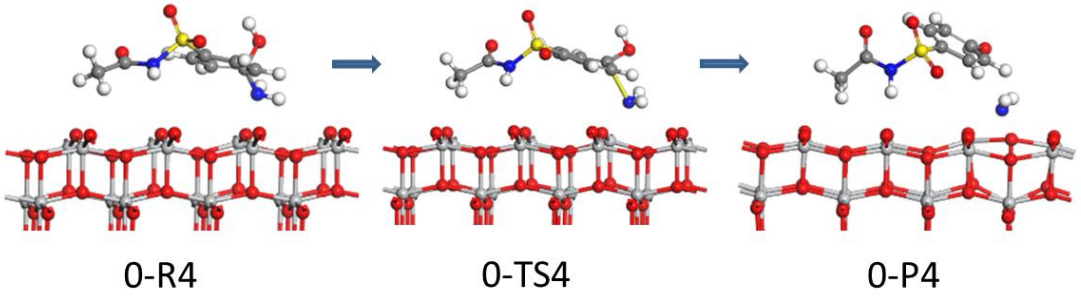
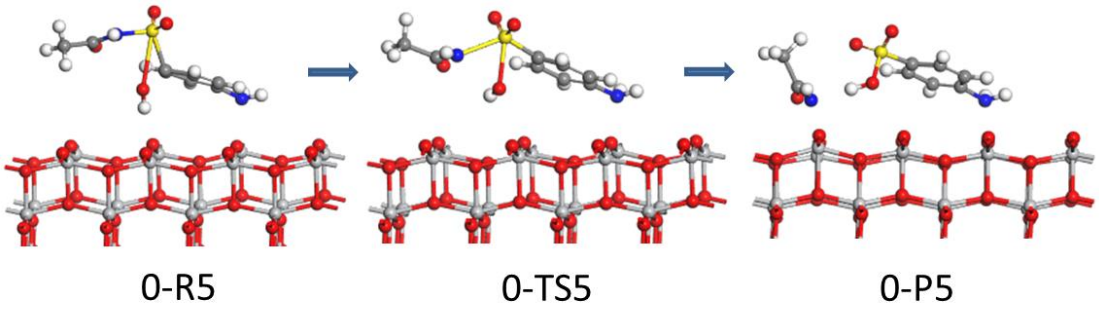



**Figure S7.** The configuration of reactants, transition states and products involved in the path4 process on （001）surface.

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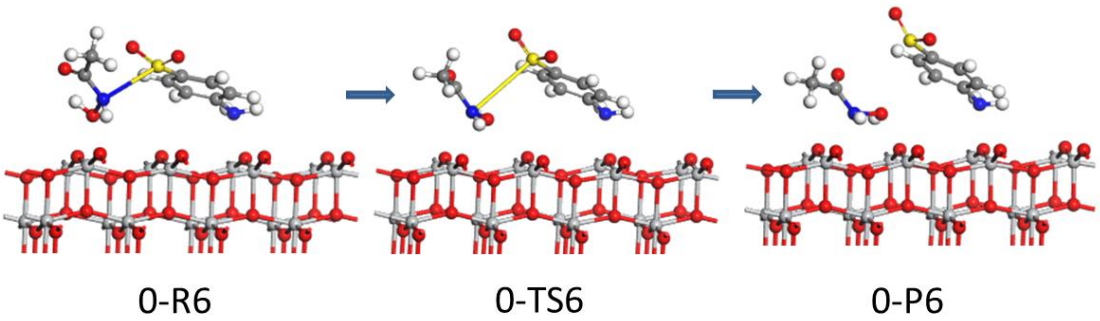
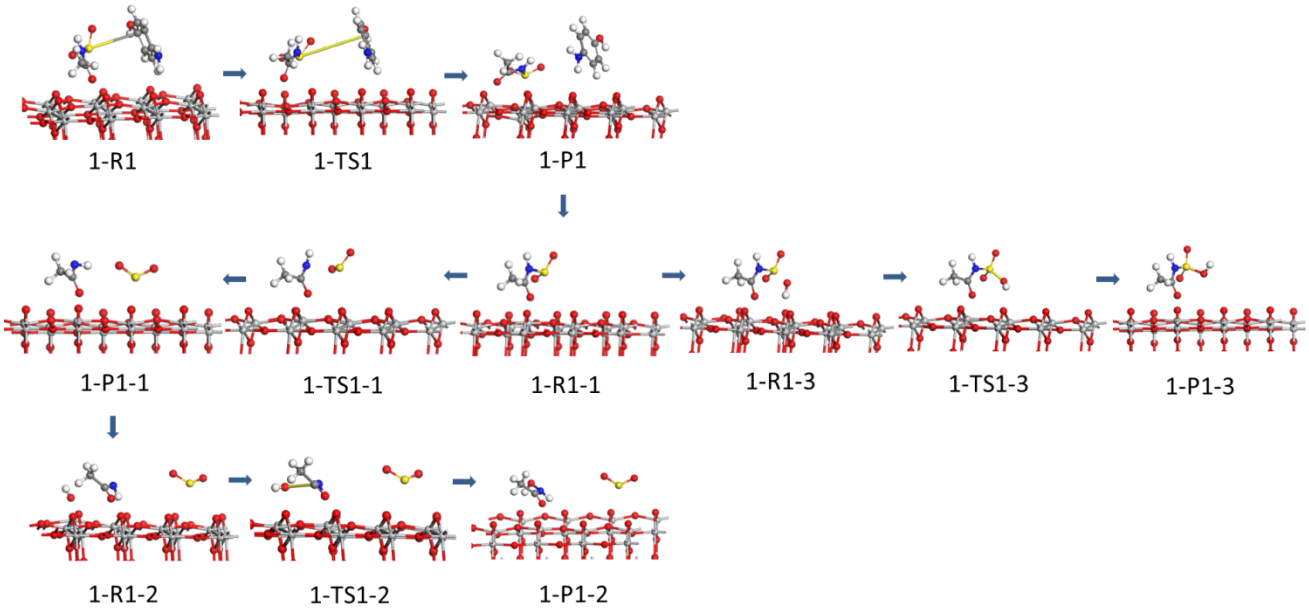



**Figure S9.** The configuration of reactants, transition states and products involved in the path6 process on （001）surface.

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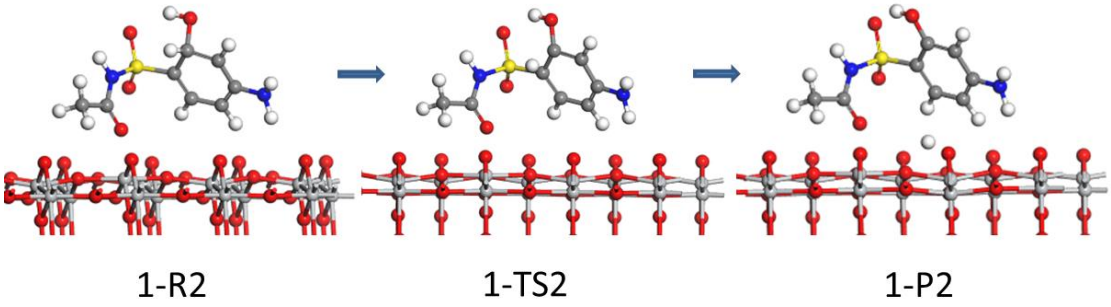


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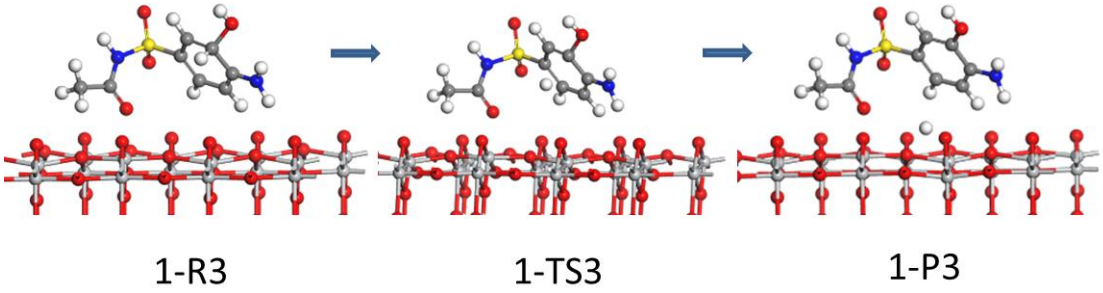


**Figure S12.** The configuration of reactants, transition states and products involved in the path3 process on （101）surface.

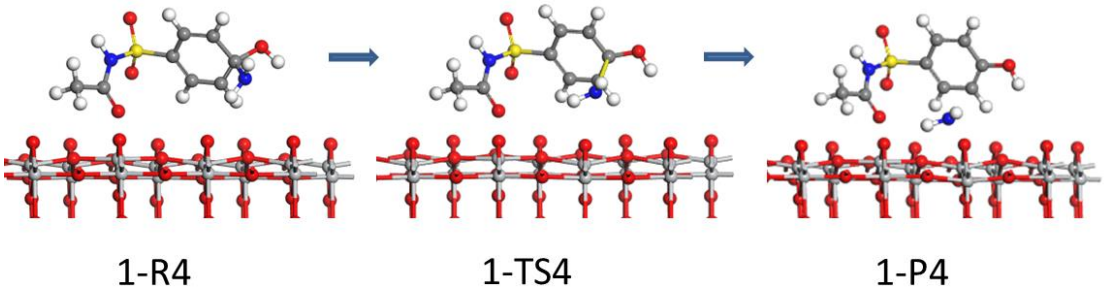


**Figure S13.** The configuration of reactants, transition states and products involved in the path4 process on （101）surface.

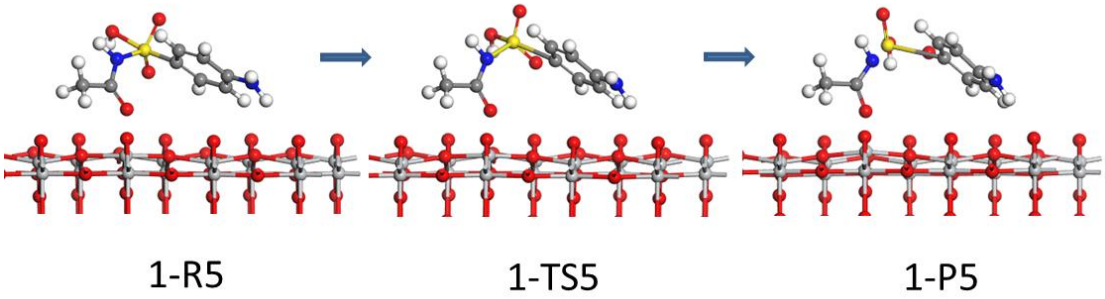


**Figure S14.** The configuration of reactants, transition states and products involved in the path5 process on （101）surface.

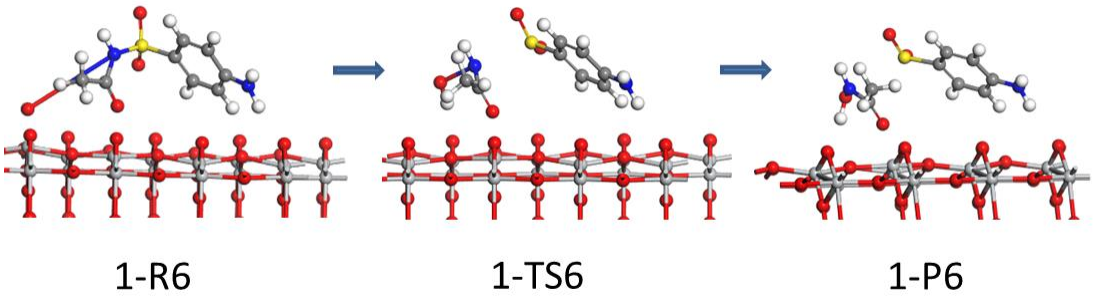


**Figure S15.** The configuration of reactants, transition states and products involved in the path6 process on （101）surface.

## 2. Tables

**Table S1.** The relative energies in the process of different SAC degradation on $TiO_2$ (001) surface reaction paths calculated at PBE+U+D3 level and corrected using more accurate HSE06+D3 method.

| Pathway | Intermediate and transition states | $\triangle E_{PBE+U+D3}$ Kcal/mol | $\triangle E_{HSE06+D3}$ Kcal/mol |
|---|---|---|---|
| **0-path1** | 0-R1 | 0.0 | 0.0 |
| | 0-TS1 | 4.1 | 7.7 |
| | 0-P1+0-R1-1 | -20.0 | -4.5 |
| | 0-TS1-1 | 21.8 | 30.9 |
| | $SO_2$+0-R1-2 | -24.0 | -22.0 |
| | 0-TS1-2 | 26.5 | 24.6 |
| | 0-P1-2 | -12.0 | -60.4 |
| | 0-TS1-3 | 29.3 | 10.3 |
| | 0-P1-3 | -28.0 | -90.7 |
| **0-path2** | 0-R2 | 0.0 | 0 |
| | 0-TS2 | 39.1 | 41.1 |
| | 0-P2+·OH | -80.9 | -40.7 |
| **0-path3** | 0-R3 | 0.0 | 0.0 |
| | 0-TS3 | 15.6 | 26.1 |
| | 0-P3+·OH | -55.1 | -40.1 |
| **0-path4** | 0-R4 | 0.0 | 0.0 |
| | 0-TS4 | 34.9 | 40.5 |
| | 0-P4+·$NH_2$ | -20.9 | 23.3 |
| **0-path5** | 0-R5 | 0.0 | 0.0 |
| | 0-TS5 | 56.7 | 77.5 |
| | 0-P5+·$NH_2$ | -76.7 | -8.5 |
| **0-path6** | 0-R6 | 0.0 | 0.0 |
| | 0-TS6 | 17.5 | 14.6 |
| | 0-P6+$NH_2OH$ | -14.7 | 1.3 |

**Table S2.** The relative energies in the process of different SAC degradation on $TiO_2$ (101) surface reaction paths calculated at PBE+U+D3 level and corrected using more accurate HSE06+D3 method.

| Pathway | Intermediate and transition states | $\triangle E_{PBE}$ Kcal/mol | $\triangle E_{XC\text{-}functional}$ Kcal/mol |
|---|---|---|---|
| **1-path1** | 1-R1 | 0.0 | 0.0 |
| | 1-TS1 | 31.9 | 39.2 |
| | 1-P1+1-R1-1 | -0.8 | 1.2 |
| | 1-TS1-1 | 25.3 | 29.7 |
| | $SO_2$+1-R1-2 | 12.1 | 22.1 |
| | 1-TS1-2 | 26.7 | 18.3 |
| | 1-P1-2 | -34.5 | -103.0 |
| | 1-TS1-3 | 26.7 | 22.0 |
| | 1-P1-3 | 11.9 | 9.5 |
| **1-path2** | 1-R2 | 0.0 | 0.0 |
| | 1-TS2 | 37.7 | 37.0 |
| | 1-P2+·OH | -68.6 | -31.3 |
| **1-path3** | 1-R3 | 0.0 | 0.0 |
| | 1-TS3 | 27.3 | 36.9 |
| | 1-P3+·OH | -60.7 | -28.8 |
| **1-path4** | 1-R4 | 0.0 | 0.0 |
| | 1-TS4 | 25.5 | 23.4 |
| | 1-P4+·$NH_2$ | -16.9 | 16.5 |
| **1-path5** | 1-R5 | 0.0 | 0.0 |
| | 1-TS5 | 45.8 | 56.8 |
| | 1-P5+·$NH_2$ | -77.0 | -27.0 |
| **1-path6** | 1-R6 | 0.0 | 0.0 |
| | 1-TS6 | 64.9 | 90.8 |
| | 1-P6+$NH_2OH$ | -49.9 | 25.1 |

**Table S3.** The adsorption energies of SAC adsorbed on $TiO_2$ surfaces in vacuum calculated using PBE+U+D3 method.

| $TiO_2$ (001) | | $TiO_2$ (101) | |
|---|---|---|---|
| Structures | $E_{ads}$(ev) | Structures | $E_{ads}$(ev) |
| CA0 | -1.416 | CA1 | -0.973 |
| CB0 | -4.153 | CB1 | -1.445 |
| CC0 | -1.662 | CC1 | -0.726 |
| CD0 | -1.812 | CD1 | -0.682 |
| CE0 | -1.552 | CE1 | -0.912 |
| CF0 | -3.972 | CF1 | -0.861 |