Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics


# Supporting Information

Table S1 Mulliken charges of each metal atoms in the most stable structures of adsorbed pure $Ag_n$ and pure $Pd_n$ clusters at the perfect and defective anatase $TiO_2$(101) surfaces.

| | | Atoms in clusters | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Pd1 | Pd2 | Pd3 | Pd4 | Pd5 | sum[a] | Ag1 | Ag2 | Ag3 | Ag4 | Ag5 | sum[b] |
| Perfect | $Pd_1$ | 0.09 | | | | | 0.09 | | | | | | |
| | $Pd_2$ | 0.16 | 0.09 | | | | 0.25 | | | | | | |
| | $Pd_3$ | 0.11 | 0.13 | 0.12 | | | 0.36 | | | | | | |
| | $Pd_4$ | 0.1 | 0.16 | 0.1 | -0.27 | | 0.09 | | | | | | |
| | $Pd_5$ | 0.01 | -0.03 | 0.05 | -0.16 | 0.24 | 0.11 | | | | | | |
| | $Ag_1$ | | | | | | | 0.58 | | | | | 0.58 |
| | $Ag_2$ | | | | | | | 0.22 | 0.05 | | | | 0.27 |
| | $Ag_3$ | | | | | | | 0.21 | 0.21 | 0.09 | | | 0.51 |
| | $Ag_4$ | | | | | | | 0.3 | 0.3 | 0.27 | 0.07 | | 0.94 |
| | $Ag_5$ | | | | | | | 0.09 | 0.14 | 0.15 | 0.05 | 0.19 | 0.62 |
| Defective | $Pd_1$ | -0.18 | | | | | -0.18 | | | | | | |
| | $Pd_2$ | -0.03 | -0.03 | | | | -0.06 | | | | | | |
| | $Pd_3$ | 0.07 | 0.07 | -0.14 | | | 0 | | | | | | |
| | $Pd_4$ | -0.18 | -0.05 | -0.05 | -0.12 | | -0.4 | | | | | | |
| | $Pd_5$ | -0.17 | -0.04 | -0.03 | 0 | -0.13 | -0.37 | | | | | | |
| | $Ag_1$ | | | | | | | 0.05 | | | | | 0.05 |
| | $Ag_2$ | | | | | | | 0.16 | 0.16 | | | | 0.32 |
| | $Ag_3$ | | | | | | | 0.16 | 0.16 | 0.12 | | | 0.44 |
| | $Ag_4$ | | | | | | | 0.13 | 0.13 | 0.12 | 0.04 | | 0.42 |
| | $Ag_5$ | | | | | | | 0.01 | 0.14 | 0.14 | 0.03 | 0.06 | 0.38 |

[a] the total charge of adsorbed $Pd_n$ cluster.

[b] the total charge of adsorbed $Ag_n$ cluster.

Table S2 Mulliken charges of each metal atoms in the most stable structures of adsorbed pure $Ag_1$ and $Pd_1Ag_1$ dimer at perfect and defective anatase $TiO_2$(101) surfaces by GGA (GGA+*U*) calculation.

| | Perfect | | | Defective | | |
|---|---|---|---|---|---|---|
| | Pd1 | Ag1 | total charge | Pd1 | Ag1 | total charge |
| $Ag_1$ | - | 0.58 (0.55) | 0.58 (0.55) | - | 0.05 (0.08) | 0.05 (0.08) |
| $Pd_1Ag_1$ | -0.12 (-0.18) | 0.28 (0.24) | 0.16 (0.06) | -0.19 (-0.21) | 0.23 (0.26) | 0.04 (0.05) |