Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# An automated reaction route mapping for the reaction of NO and active species on $Ag_4$ cluster in zeolite

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Table S1 convergence of cutoff energy for representative structures

| | $E_{400eV}$ (eV) | $E_{500eV}$ (eV) | $E_{600eV}$ (eV) |
|---|---|---|---|
| $Ag_4(H)(OOH)$ (EQ5) | -888.2 | -886.5 | -886.8 |
| $Ag_4 + O_2 + H_2$ (EQ48) | -887.6 | -885.9 | -886.2 |
| $\Delta E$ (EQ5–EQ48) | -0.60 | -0.58 | -0.58 |
| $Ag_4 + 3H_2 + NO$ (EQ4) | -904.3 | -902.6 | -903.0 |
| $Ag_4(ONH_2) + 2H_2$ (EQ99) | -905.6 | -903.9 | -904.3 |
| $\Delta E$ (EQ4–EQ99) | -1.3 | -1.3 | -1.3 |

Table S2 convergence of k-point mesh for representative structures

| | $E_{1\times1\times1}$ (eV) | $E_{2\times2\times2}$ (eV) | $E_{3\times3\times3}$ (eV) |
|---|---|---|---|
| $Ag_4(H)(OOH)$ (EQ5) | -888.2 | -888.2 | -888.2 |
| $Ag_4 + O_2 + H_2$ (EQ48) | -887.6 | -887.6 | -887.6 |
| $\Delta E$ (EQ5–EQ48) | -0.60 | -0.60 | -0.60 |
| $Ag_4 + 3H_2 + NO$ (EQ4) | -904.3 | -904.4 | -904.4 |
| $Ag_4(ONH_2) + 2H_2$ (EQ99) | -905.6 | -905.7 | -905.7 |
| $\Delta E$ (EQ4–EQ99) | -1.3 | -1.3 | -1.3 |

Table S3 Comparison before/after the optimization of lattice constants (their volumes were fixed)

| | $a$ (Å) | $b$ (Å) | $c$ (Å) | $\alpha$ (°) | $\beta$ (°) | $\gamma$ (°) |
|---|---|---|---|---|---|---|
| Experiment | 13.675 | 13.675 | 14.767 | 90 | 90 | 120 |
| CHA (Si only) | 13.675 | 13.675 | 14.767 | 90 | 90 | 120 |
| $Ag_4(H)(OOH)$ (EQ5) | 13.669 | 13.684 | 14.757 | 89.66 | 90.03 | 119.96 |
| $Ag_4 + O_2 + H_2$ (EQ48) | 13.675 | 13.675 | 14.767 | 90 | 90 | 120 |
| $Ag_4 + 3H_2 + NO$ (EQ4) | 13.675 | 13.675 | 14.767 | 90 | 90 | 120 |
| $Ag_4(ONH_2) + 2H_2$ (EQ99) | 13.675 | 13.675 | 14.767 | 90 | 90 | 120 |

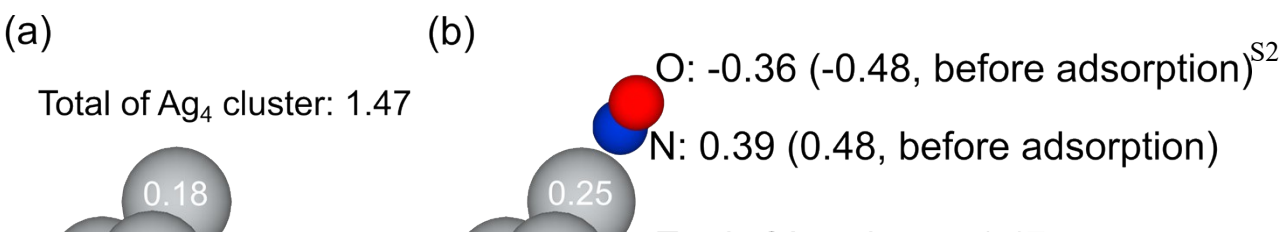

Figure S1 Bader charge analysis for $Ag_4$ cluster in CHA zeolite (a) before/ (b) after NO adsorption. Color codes: Si (yellow), Al (green), O (red), N (blue), and Ag (silver).