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Supporting Informations

The Adsorption and Growth of $Ag_n(n = 1\sim4)$ Clusters on Cubic, Monoclinic, and Tetragonal ZrO_2 Surfaces: A First-Principles Study

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Fig. S1 Top view of all the adsorption configurations and the corresponding energies of Ag_n ($n=1\sim 4$) structures adsorbed on c-ZrO₂ (1 1 1) surface at all possible sites. Only the surface atoms are shown as round (red, O; white-blue, Zr, darkblue, Ag). This notation is used throughout this paper.

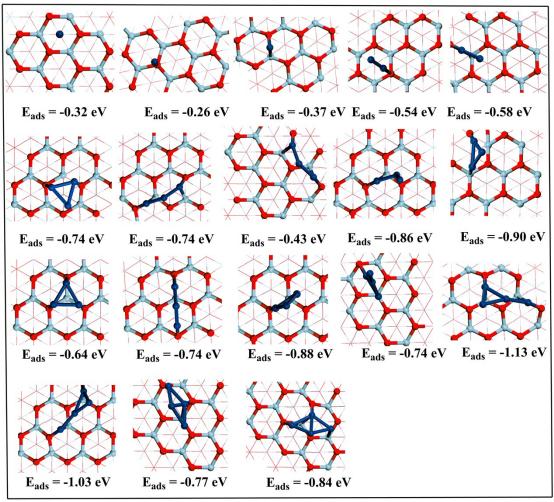


Fig. S2 Top view of all the adsorption configurations and the corresponding energies of Ag_n (n = 1 ~ 4) structures adsorbed on t-ZrO₂ (1 0 1) surface at all possible sites.

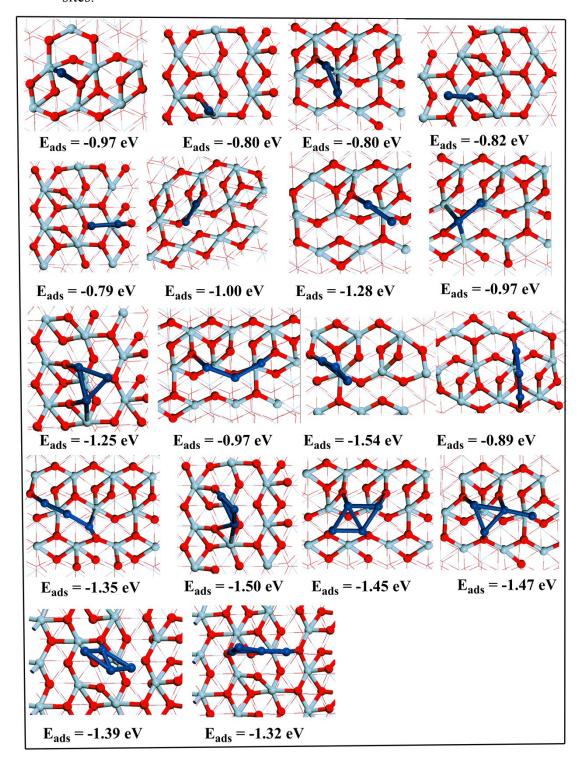


Fig. S3 Top view of all the adsorption configurations and the corresponding energies of Ag_n (n = 1 ~ 4) structures adsorbed on m-ZrO₂ ($^{\mbox{$\overline{1}$}}$ 1 1) surface at all possible sites.

