Supporting Informations

The Adsorption and Growth of Ag\textsuperscript{n}(n = 1\sim 4) Clusters on Cubic, Monoclinic, and Tetragonal ZrO\textsubscript{2} Surfaces: A First-Principles Study

Tingting Liu\textsuperscript{a}, Yan Li\textsuperscript{b, c}, Changhai Liang\textsuperscript{a}

\textsuperscript{a}School of Petroleum and Chemical Engineering, Dalian University of Technology, Panjin, 124221, P. R. China

\textsuperscript{b}School of Chemical Engineering, University of Science and Technology Liaoning, Anshan 114051, P. R. China

Corresponding person: Yan Li
E-mail: snow2007liyan@163.com
Telephone: 86-15142738951
Fax: 86-427-2631111
Fig. S1 Top view of all the adsorption configurations and the corresponding energies of Ag$_n$ ($n = 1 \sim 4$) structures adsorbed on c-ZrO$_2$ (1 1 1) surface at all possible sites. Only the surface atoms are shown as round (red, O; white-blue, Zr; dark-blue, Ag). This notation is used throughout this paper.
Fig. S2 Top view of all the adsorption configurations and the corresponding energies of Agₙ (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-ZrO$_2$ (1 1 1) surface at all possible sites.