Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information:

Mechanistic Study of Ethanol Transformation into Ethene and Acetaldehyde on Oxygenated Au-Exchanged ZSM-5 Zeolite

Yuwanda Injongkol[a,b], Thana Maihom[a,b], Saowapak Choomwattana[c], Bundet Boekfa[a,b], and Jumras Limtrakul[d]

[a]Department of Chemistry, Faculty of Liberal Arts and Science, Kasetsart University, Kamphaeng Saen Campus, Nakhon Pathom 73140, Thailand

[b] Center for Advanced Studies in Nanotechnology and Its Applications in Chemical, Food and Agricultural Industries and NANOTEC Center for Nanoscale Materials Design for Green Nanotechnology, Kasetsart University, Bangkok 10900, Thailand.

[c]Center of Data Mining and Biomedical Informatics, Faculty of Medical Technology, Mahidol University, Salaya Campus, Nakhon Pathom 73170, Thailand.

[d]Department of Materials Science and Engineering, Vidyasirimedhi Institute of Science and Technology, Rayong 21210, Thailand.

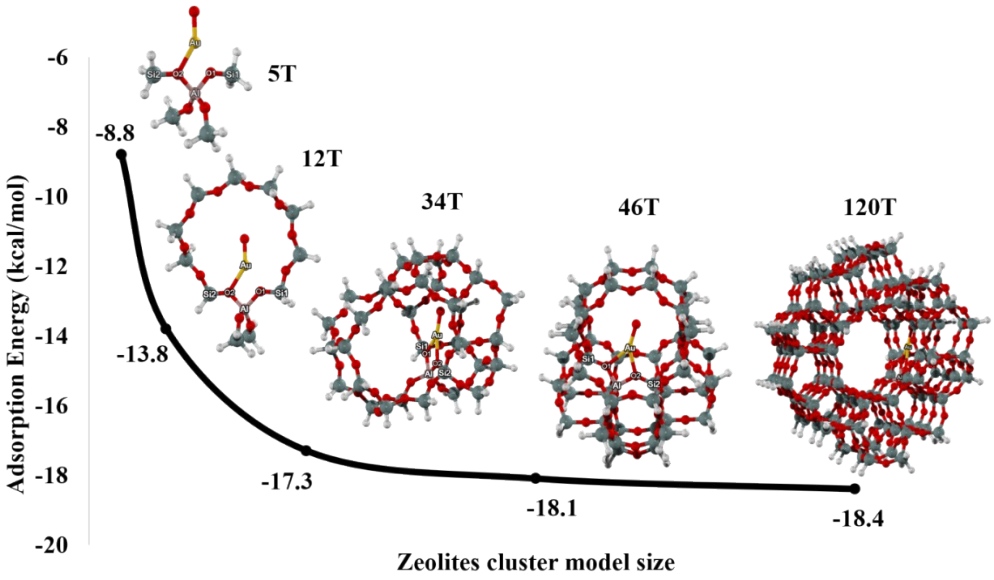


Fig. S1 The ethanol adsorption energies of the AuO/ZSM-5 as a function of the cluster model sizes.

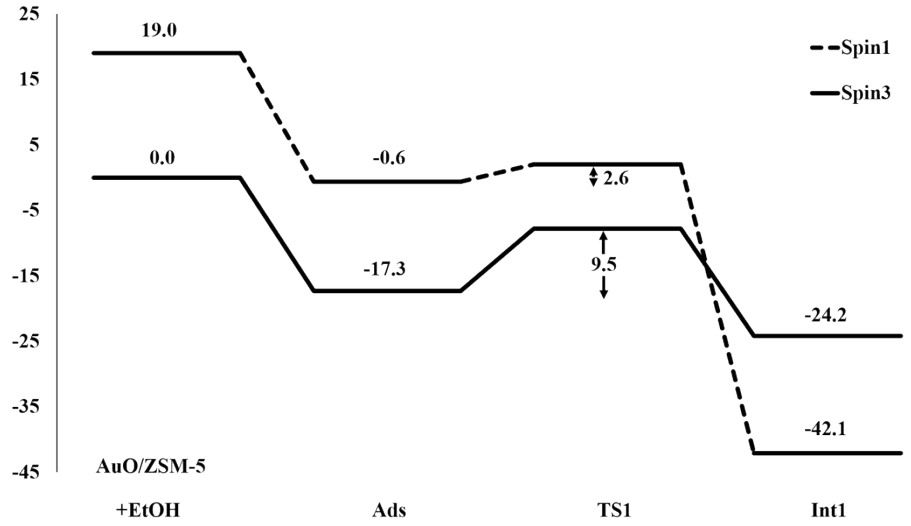


Fig. S2 Energy profile for the ethoxide-hydroxide intermediate formation on AuO/ZSM-5 for singlet state (dot line) and triplet state (solid line). Energies are in kcal/mol.

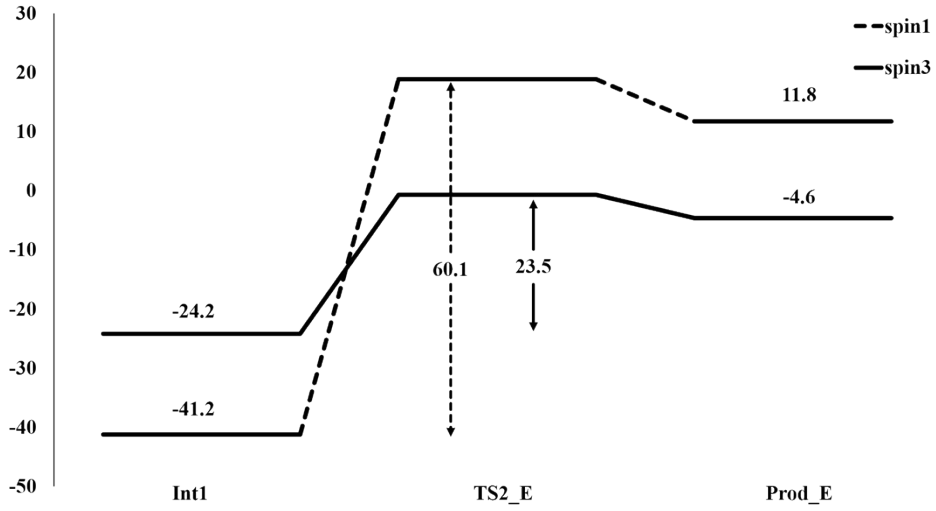


Fig. S3 Energy profile for the ethoxide-hydroxide conversion to ethene on AuO/ZSM-5 for singlet state (dot line) and triplet state (solid line). Energies are in kcal/mol.

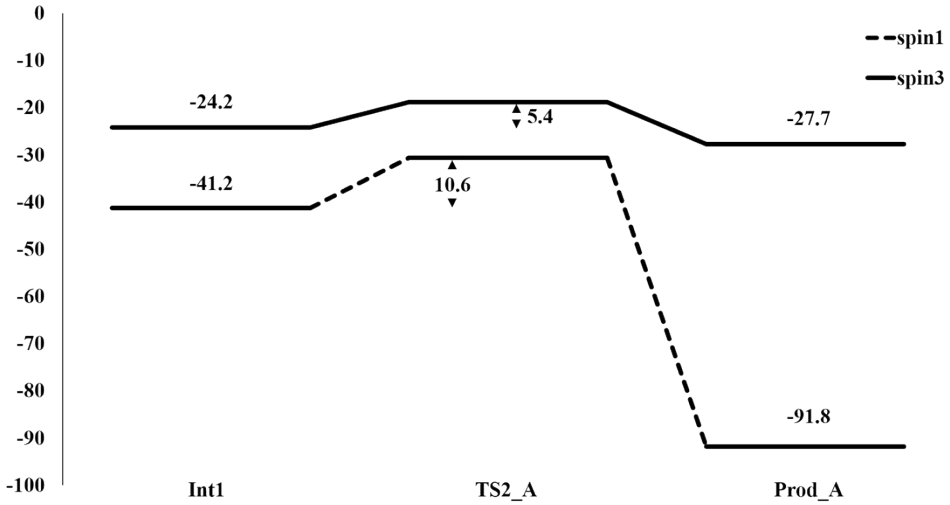
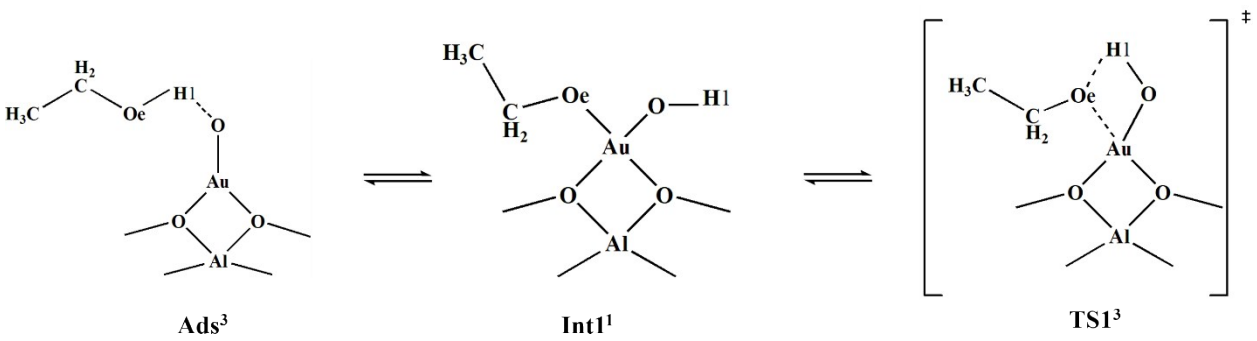
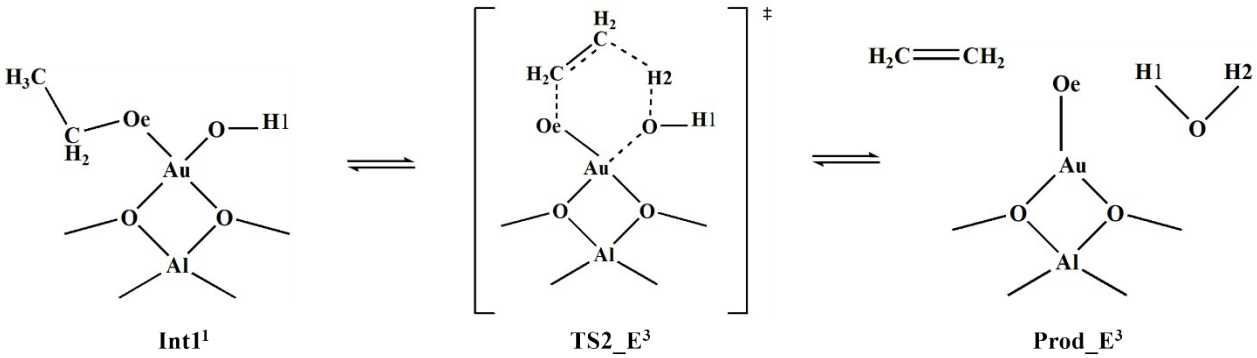


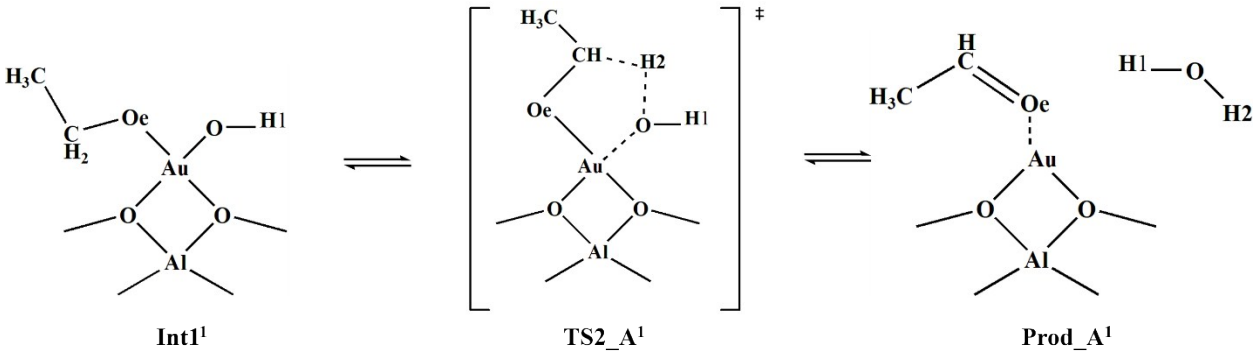
Fig. S4 Energy profile for the ethoxide-hydroxide conversion to acetaldehyde on AuO/ZSM-5 for singlet state (dot line) and triplet state (solid line). Energies are in kcal/mol.



(a)



(b)



(c)

Fig. S5 The reaction mechanisms with two-dimensional chemical structure of the ethoxide-hydroxide intermediate formation (a) and the conversion of the ethoxide-hydroxide to ethene (b) and acetaldehyde (c).

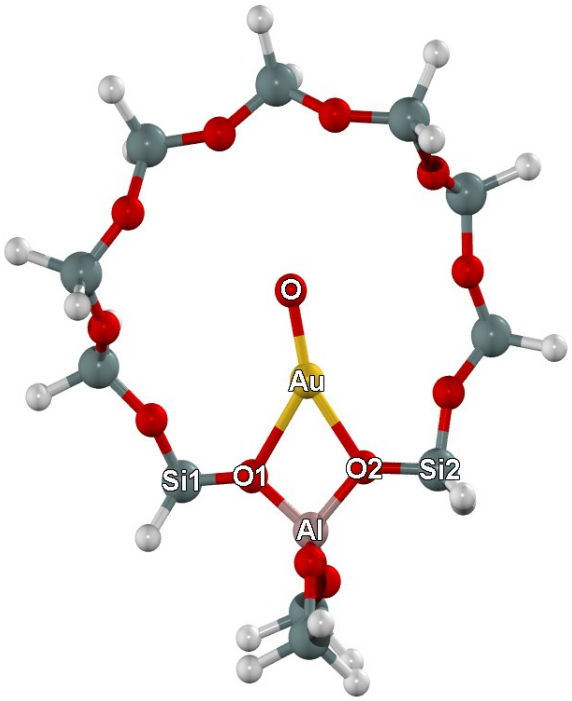


Fig. S5 The 12T cluster model of AuO/ZSM-5 zeolite.