Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Structure-activity relationships in the production of olefins from alcohols and ethers: A first-principles theoretical study

Supporting Information

S01: Energy diagrams of reaction pathways for the (ethyl) alcohol dehydration via E1 and E2 mechanisms, on five metal oxide clusters studied: Alox, Gaox, Inox, Ga-Alox and In-Alox. The dehydration of 1-propanol, 2-propanol and t-butanol (not shown) evolved through the same pathways. Adsorbed species are denoted with an asterisk (*). Transition states are denoted with a double dagger (‡).

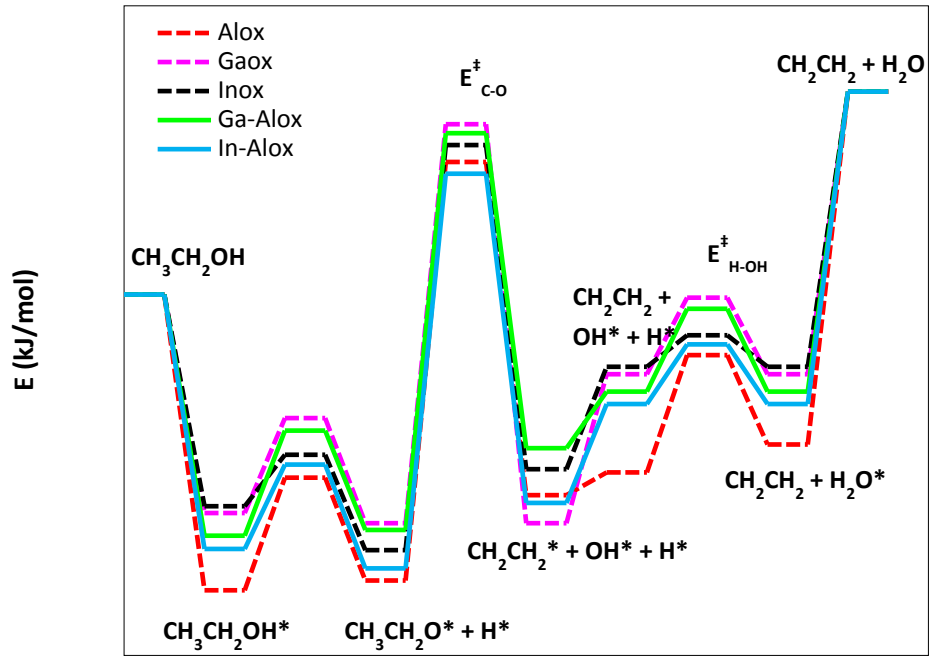

Figure 1: Ethanol dehydration reaction pathway for the E1 mechanism on five metal oxide catalysts investigated in this work.

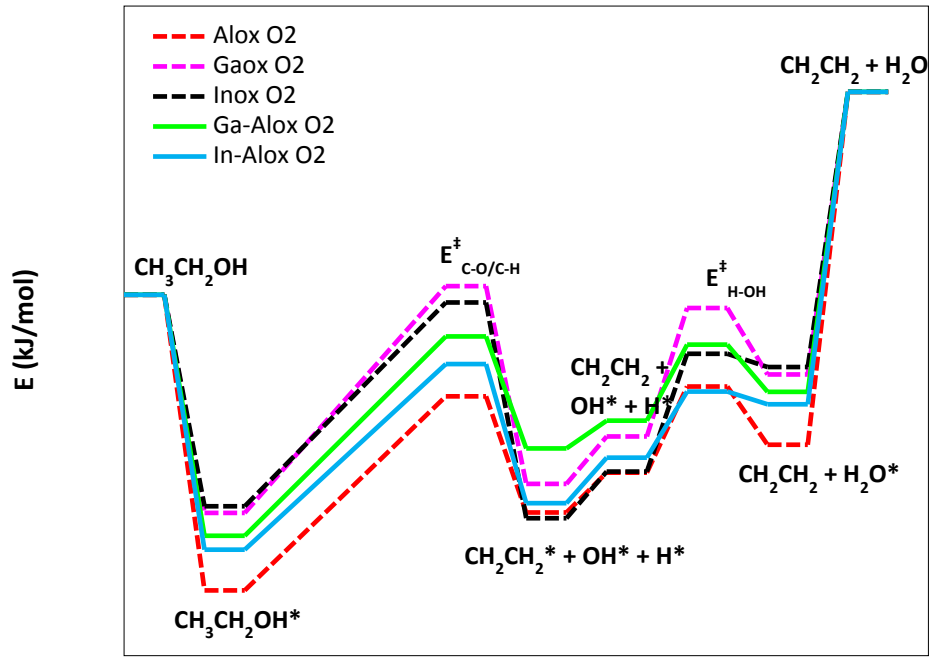

Figure 2: Ethanol dehydration reaction pathway for the E2 mechanism, involving twofold-coordinated (O2) H^{β} abstarctions site, on five metal oxide catalysts investigated in this work.

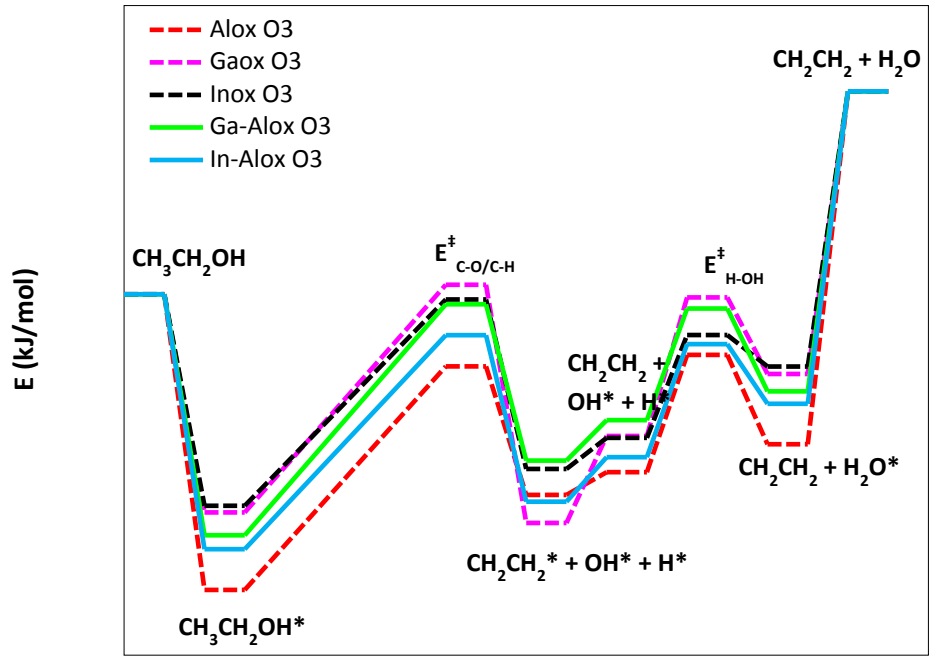

Figure 3: Ethanol dehydration reaction pathway for the E2 mechanism, involving threefold-coordinated (O3) H^{β} abstractions site, on five metal oxide catalysts investigated in this work.

S02: Energy diagrams of reaction pathways for diethyl ether (DEE) decomposition via the E1-like and E2-like mechanisms, on five metal oxide clusters studied: Alox, Gaox, Inox, Ga-Alox and In-Alox. The decomposition of di-1-propyl ether, di-2-propyl ether and di-tert-butyl ether (not shown) evolved through the same pathways. Adsorbed species were denoted with an asterisk (*). Transition states were denoted with a double dagger (‡).

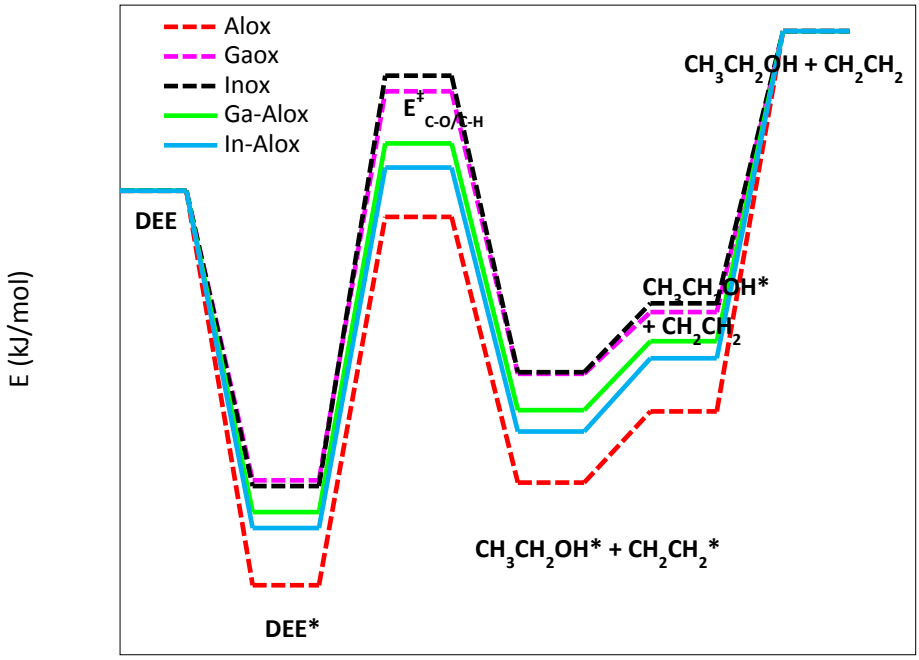

Figure 4: Diethyl ether decomposition reaction pathway for the E1-like mechanism on five metal oxide catalysts investigated in this work.

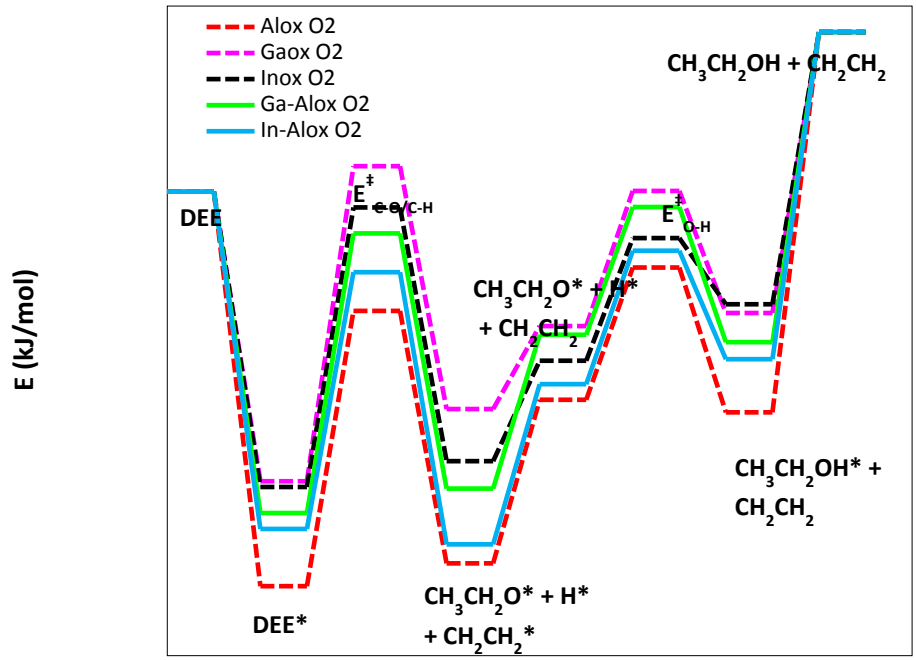

Figure 5: Diethyl ether decomposition reaction pathway for the E2-like mechanism, involving twofold-coordinated (O2) H abstarctions site, on five metal oxide catalysts investigated in this work.

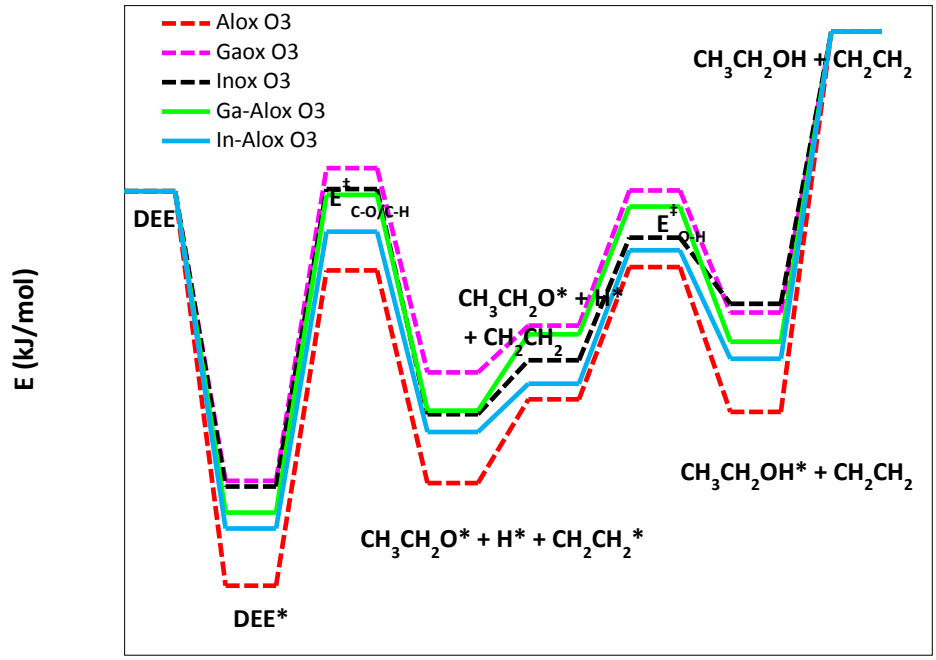

Figure 6: Diethyl ether decomposition reaction pathway for the E2-like mechanism, involving threefold-coordinated (O3) H abstarctions site, on five metal oxide catalysts investigated in this work.