Electronic Supplementary Material

Yttria-stabilized zirconia of balanced acid–base pair for selective dehydration of 4-methyl-2-pentanol to 4-methyl-1-pentene

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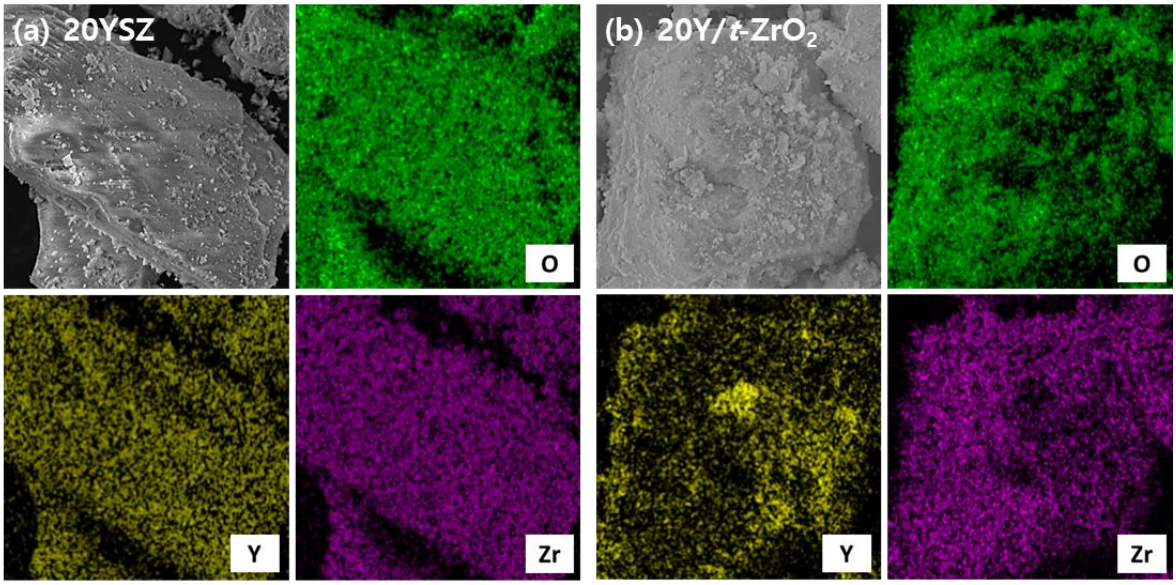

Figure S1. FE-SEM images and elemental mapping images (O, Y, and Zr) of (a) 20YSZ and (b) 20Y/*t*-ZrO_2.

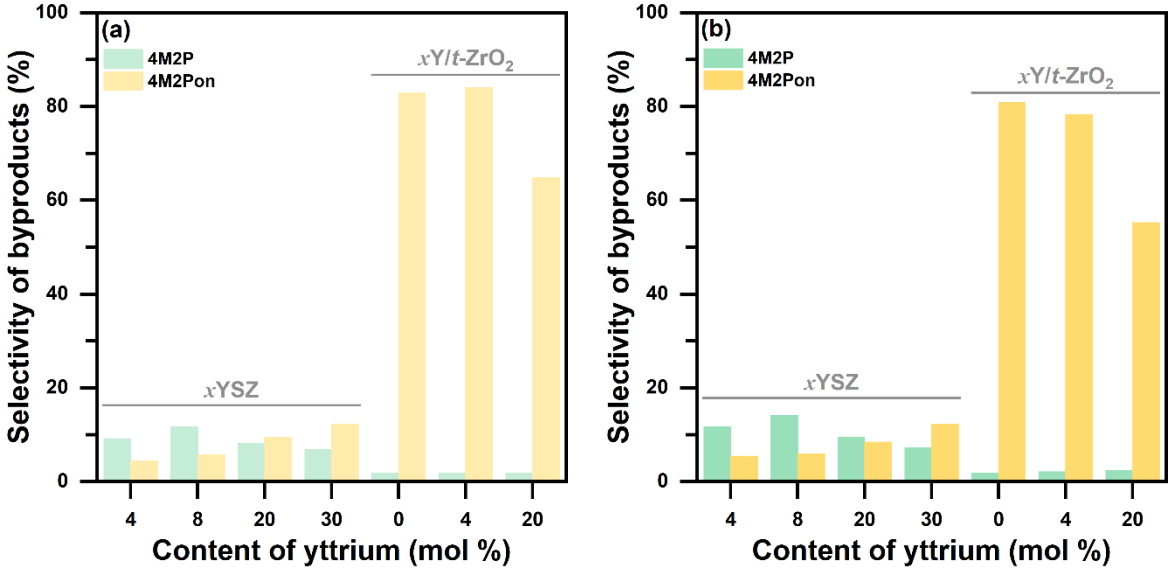

Figure S2. Selectivity of by-products such as 4M2P and 4M2Pon in 4M2Pol dehydration at (a) 350 °C and (b) 375 °C.

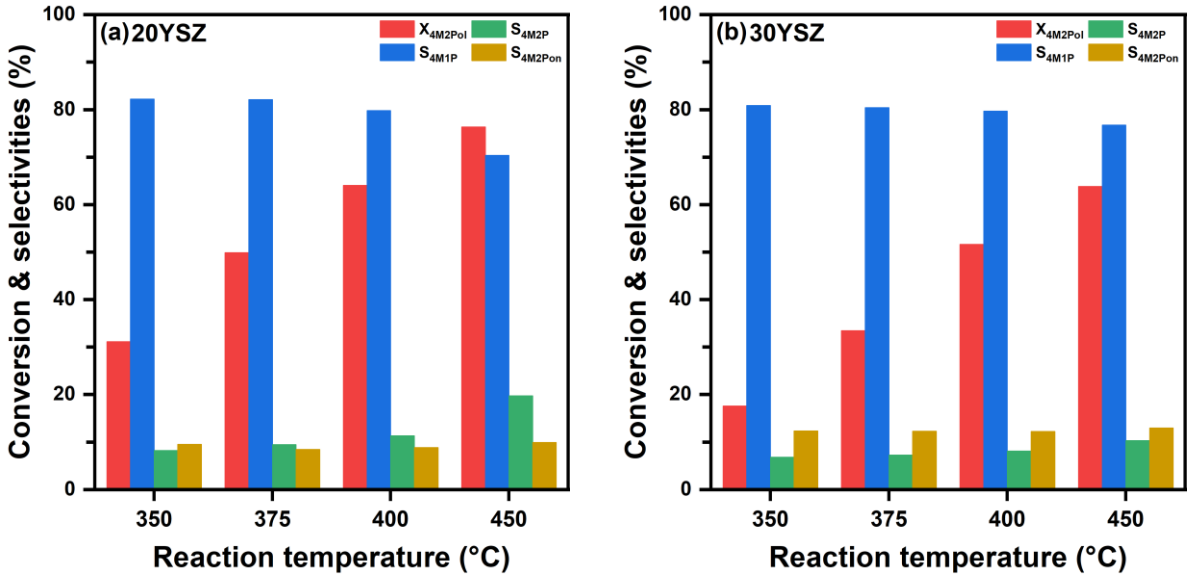

Figure S3. 4M2P conversion and product selectivity in 4M2Pol dehydration over (a) 20YSZ and (b) 30YSZ at 350 to 450 °C.

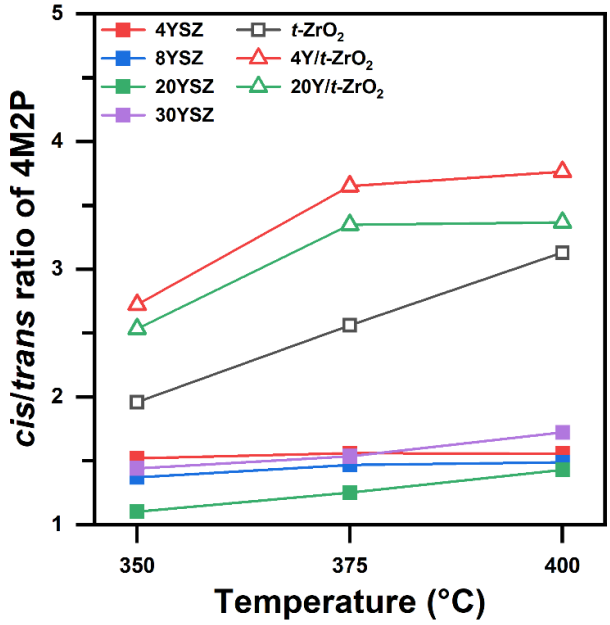

Figure S4. Ratio of *cis*- to *trans*-4M2P at 350, 375, and 400 °C over the co-precipitated *x*YSZ (*x* = 4, 8, 20, and 30) and impregnated *x*Y/*t*-ZrO_2 (*x* = 4 and 20) catalysts along with bare *t*-ZrO_2.

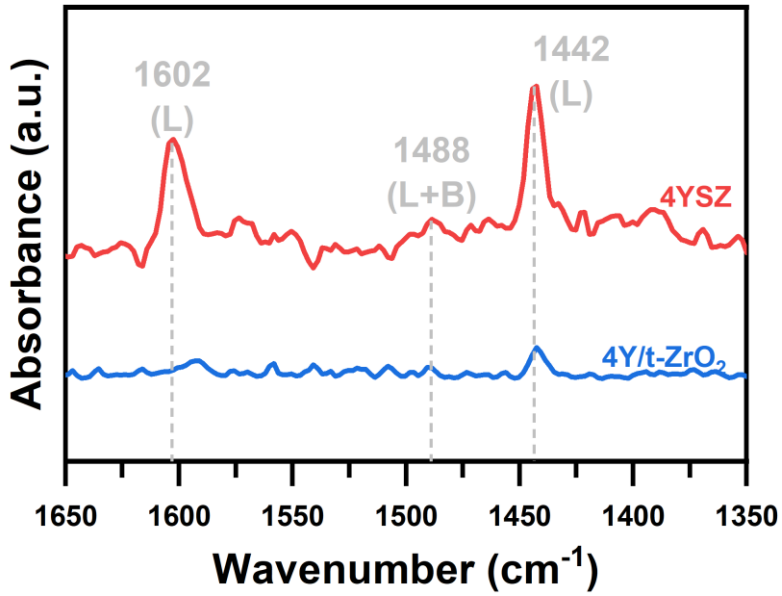

Figure S5. Pyridine-chemisorbed FT-IR spectra of the catalysts 4YSZ and 4Y/*t*-ZrO_2.

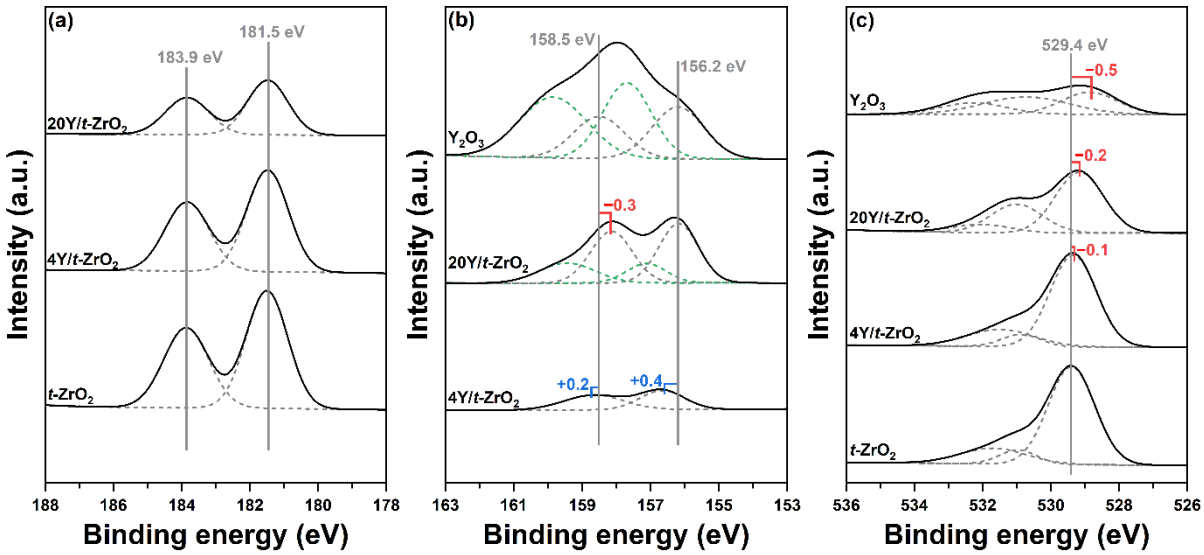

Figure S6. XPS spectra of the impregnated Y/*t*-ZrO_2 catalysts in the core levels of (a) Zr 3d, (b) Y 3d, and (c) O 1s. The spectra of *t*-ZrO_2 and/or Y_2O_3 are added for comparison.

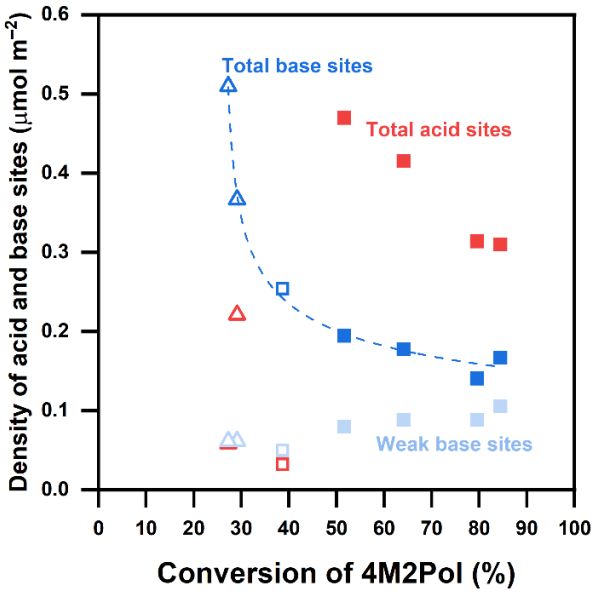

Figure S7. Correlation of 4M2Pol conversion with the surface density of total acid sites, weak base sites, and total base sites of *x*YSZ (filled squares), *x*Y/*t*-ZrO_2 (open triangles), and bare *t*-ZrO_2 (open squares).

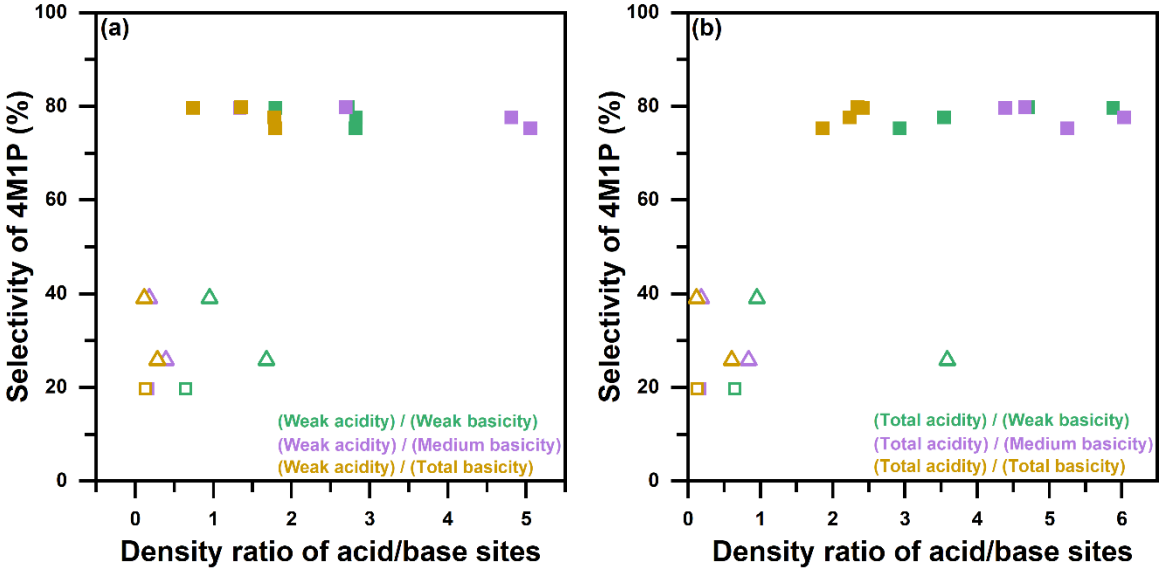

Figure S8. Correlation of 4M1P selectivity with various surface density ratios. (a) Weak acidity to weak, medium, and total basicity. (b) Total acidity to weak, medium, and total basicity for *x*YSZ (filled squares), *x*Y/*t*-ZrO_2 (open triangles), and bare *t*-ZrO_2 (open squares).

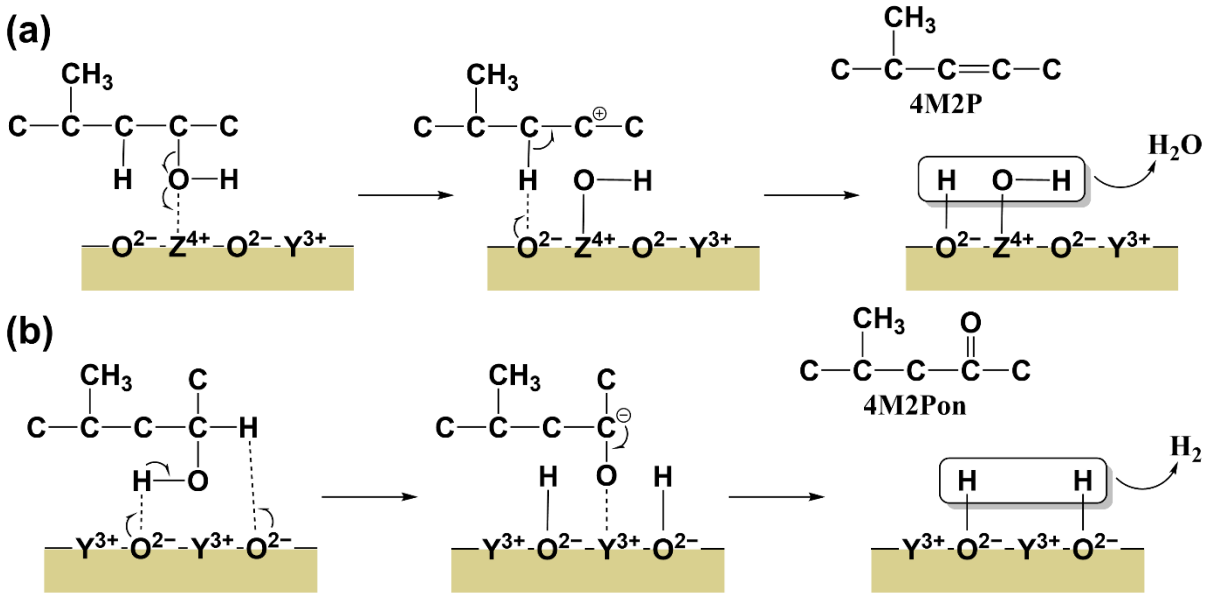

Figure S9. Plausible mechanism on the conversion of 4M2Pol. (a) Formation of 4M2P via E1 mechanism over YSZ. (b) Formation of 4M2Pon via dehydrogenation mechanism over YSZ.