

Supplementary for

DFT Insights into Crystal Plane Effects of Molybdenum Phosphide (MoP) on the Catalytic Performance in Deoxygenation of Palmitic Acid

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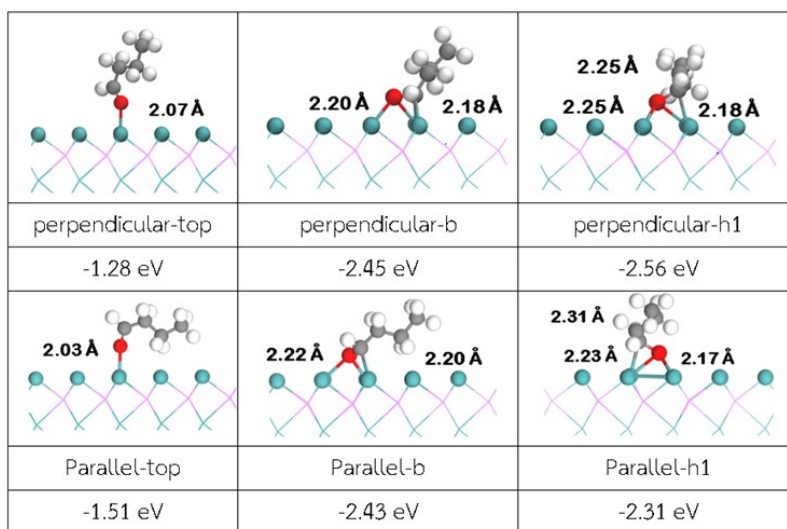
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The adsorption of butanal and butanol on MoP (001) and MoP (101) surfaces

➤ Fig. S1. Optimized structures of butanal adsorption on MoP (001) surface



➤ Fig. S2. Optimized structures of butanol adsorption on MoP (001) surface

perpendicular-top	perpendicular-b	perpendicular-h1	perpendicular-h2
-1.34 eV	-1.25 eV	-1.42 eV	-1.31 eV
Parallel-top	Parallel-b	Parallel-h1	Parallel-h2
-1.37 eV	-1.25 eV	-1.24 eV	-1.25 eV

➤ Fig. S3. Optimized structures of butanol adsorption on MoP (101) surface

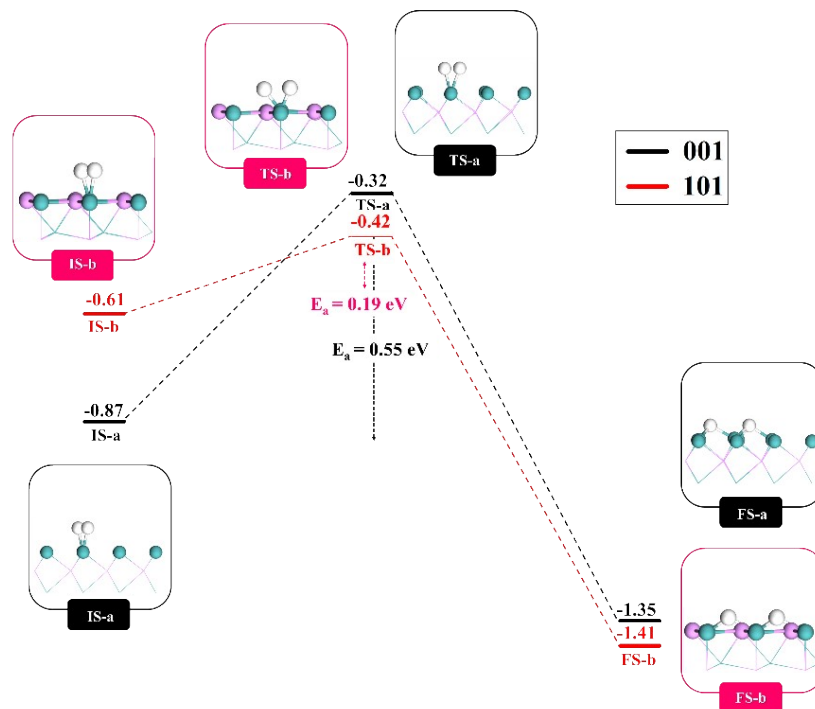
perpendicular-top	perpendicular-b	Parallel-top	Parallel-b
-1.16 eV	-1.43 eV	-1.10 eV	-1.04 eV

➤ Fig. S4. Optimized structures of butanol adsorption on MoP (101) surface

perpendicular-top	Parallel-top	Parallel-b
-1.16 eV	-1.12 eV	-1.12 eV

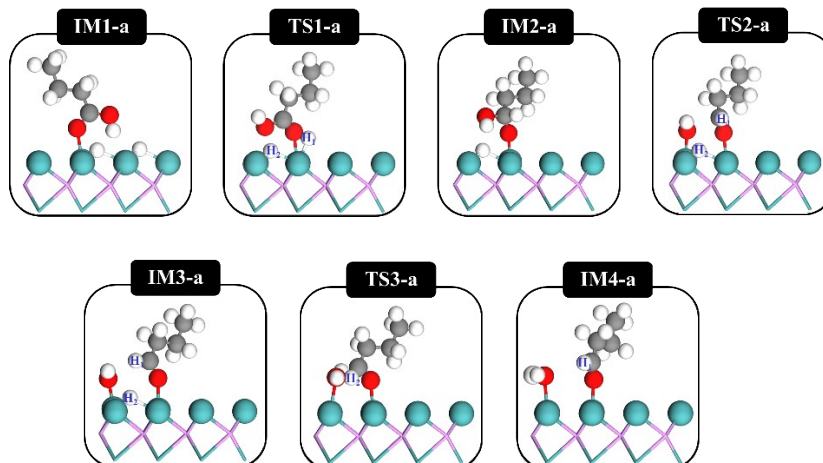
H₂ dissociation

- Fig. S5. Energy profiles and structures along the H₂ dissociation on MoP (001) and MoP (101) surfaces

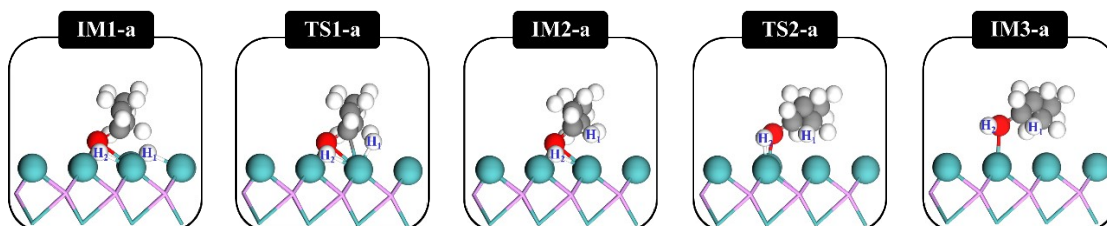


DX reaction mechanism on MoP (001) surface

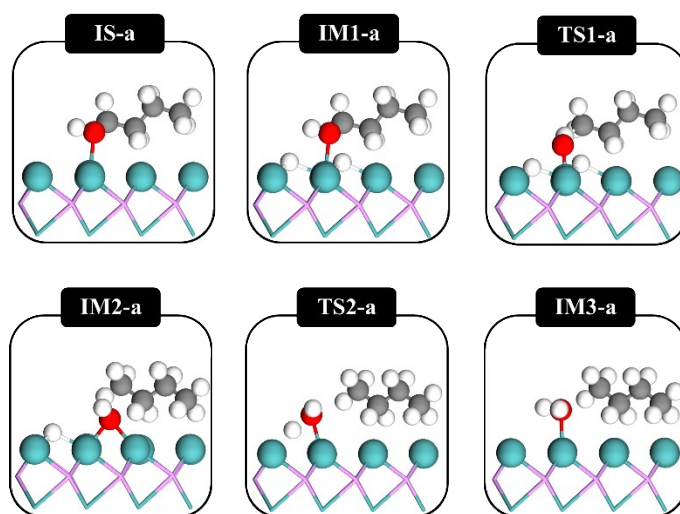
- Fig. S6. The butyric acid conversion to butanal pathway on MoP (001) surface



➤ Fig. S7. The butanal conversion to butanol pathway on MoP (001) surface



➤ Fig. S8. The butanol conversion to butane pathway on MoP (001) surface



➤ Fig. S9. The butanal conversion to propane pathway on MoP (001) surface

