Electronic Supplementary Material (ESI) for Green Chemistry.

Room-temperature tandem conversion of cyclic alkenes into 1,2-diols using molecular oxygen and β-MnO_2 heterogeneous catalyst

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Control experiments

β-MnO_2-water hydration reaction: 0.05 g of the β-MnO_2 catalyst, 5 mL of acetonitrile, 2.5 mL of water and 100 μL cyclohexene oxide was mixed together for hydration reaction at a stirring rate of 600 rpm in a 25 mL Teflon-lined stainless-steel autoclave. Isobutyric acid-water hydration reaction: 400 μL isobutyric acid, 5 mL of acetonitrile, 2.5 mL of water and 100 μL cyclohexene oxide was mixed together for hydration reaction at a stirring rate of 600 rpm in a 25 mL Teflon-lined stainless-steel autoclave. β-MnO_2-isobutyric acid-water hydration reaction: 0.05 g of the β-MnO_2 catalyst, 5 mL of acetonitrile, 400 μL isobutyric acid, 2.5 mL of water and 100 μL cyclohexene oxide was mixed together for hydration reaction at a stirring rate of 600 rpm in a 25 mL Teflon-lined stainless-steel autoclave.

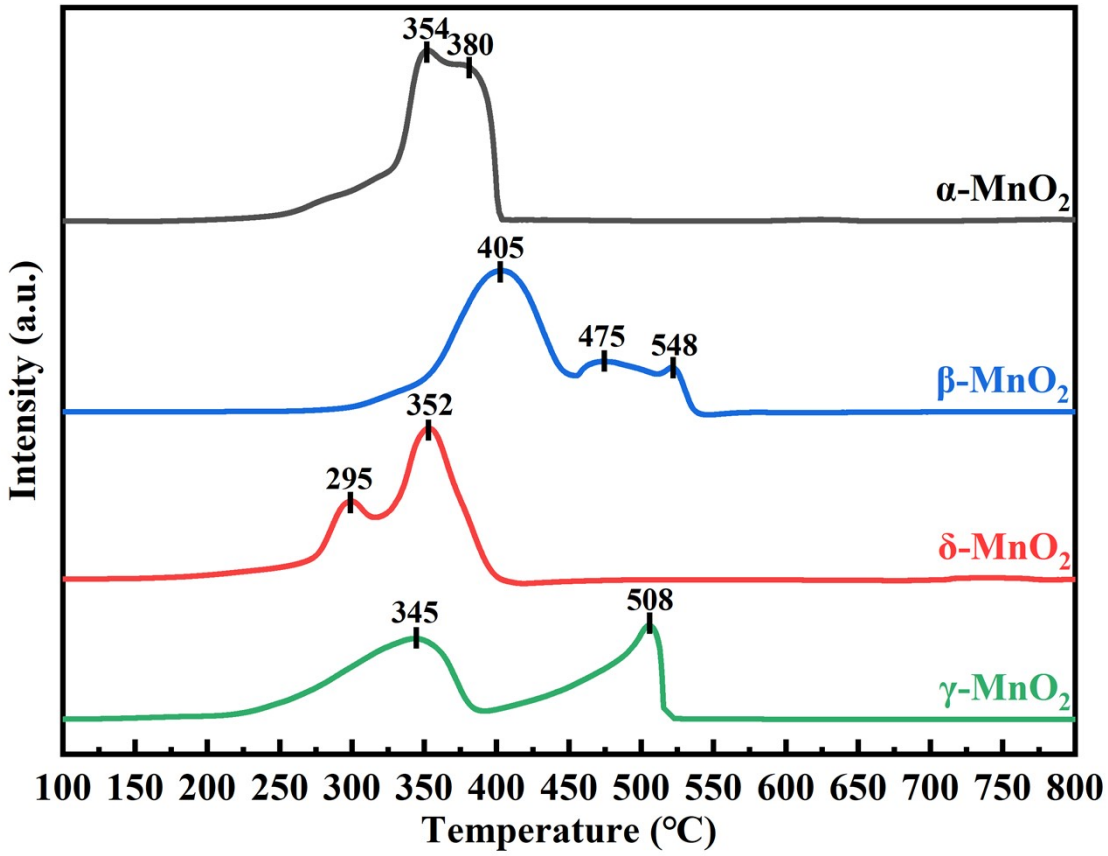

Fig. S1 H_2-TPR profiles of the four MnO_2 samples

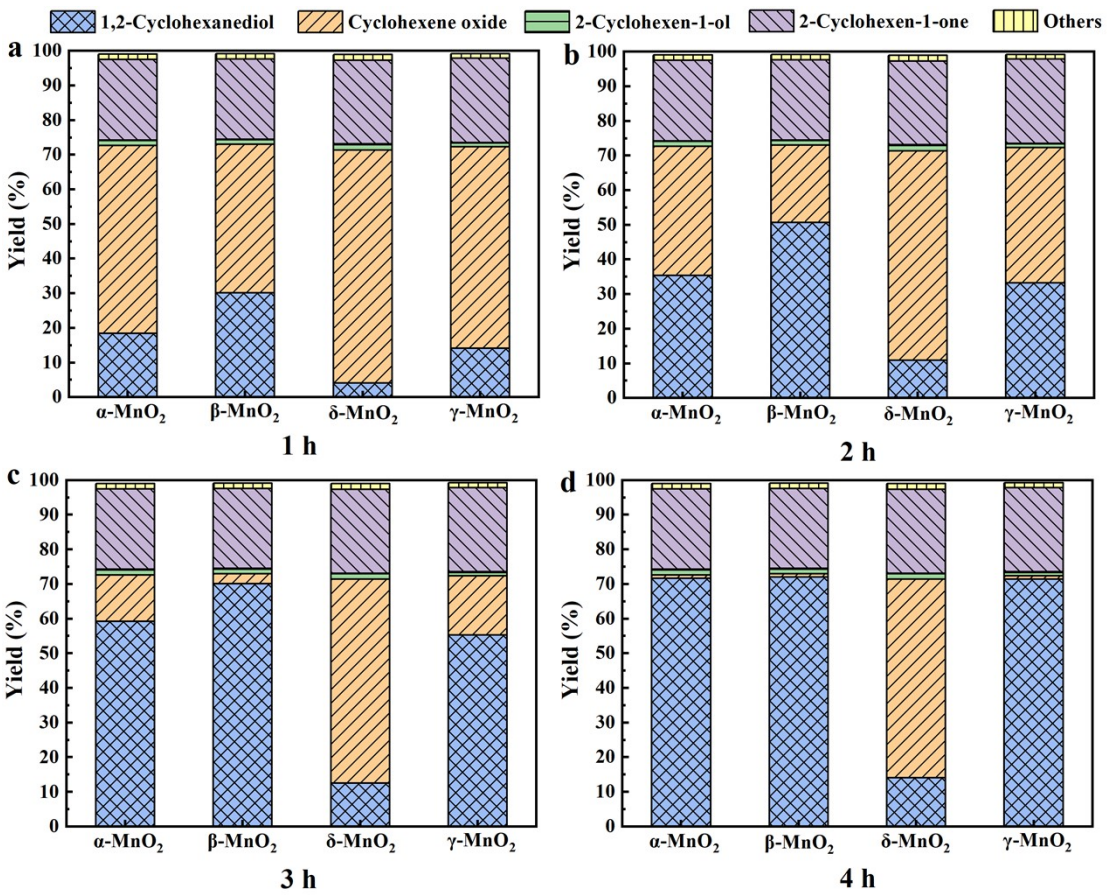

Fig. S2 Yield of the products with reaction time for tandem conversion reaction at 50 °C

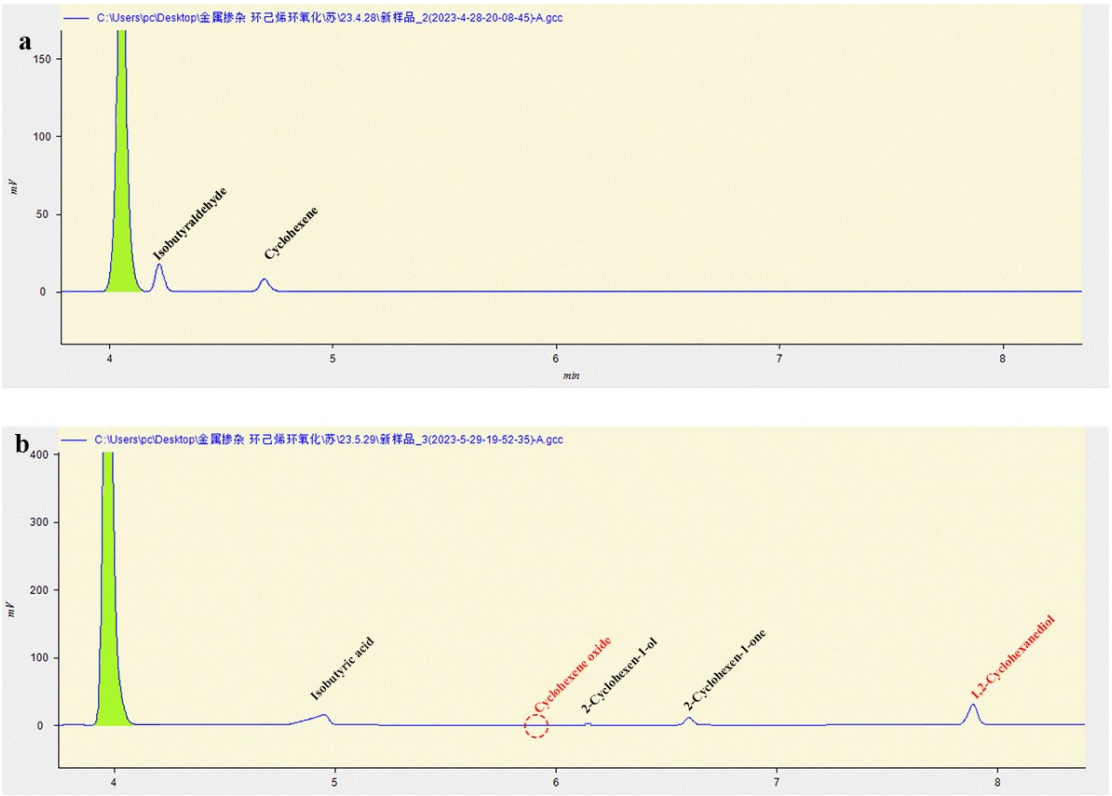

Fig. S3 Gas chromatograms for the tandem conversion reaction solutions before reaction (a) and after reaction (b)

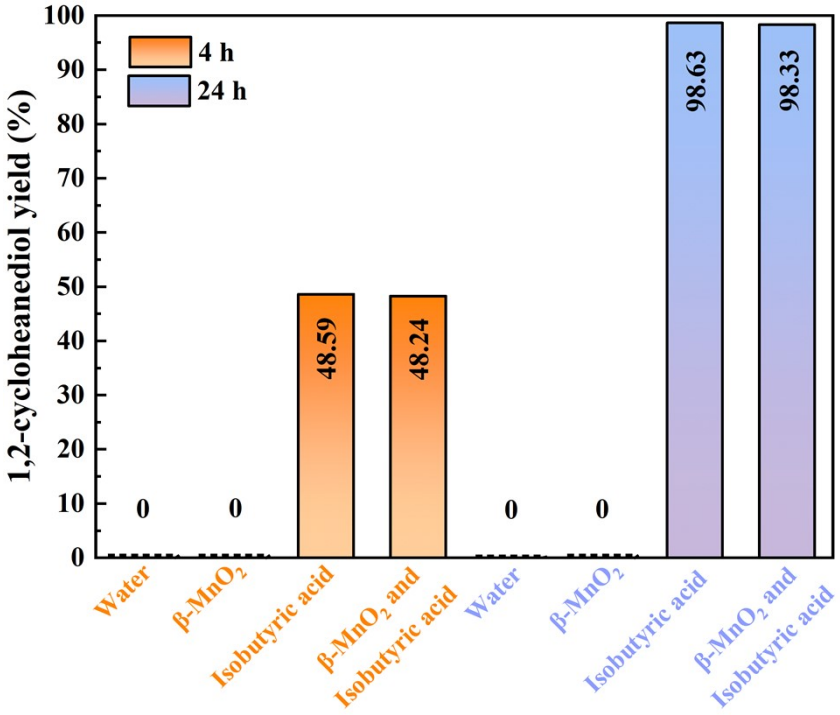

Fig. S4 Control experiments including water alone, β-MnO_2-water, isobutyric acid-water and β-MnO_2-isobutyric acid-water reaction systems for the direct hydration of cyclohexene oxide

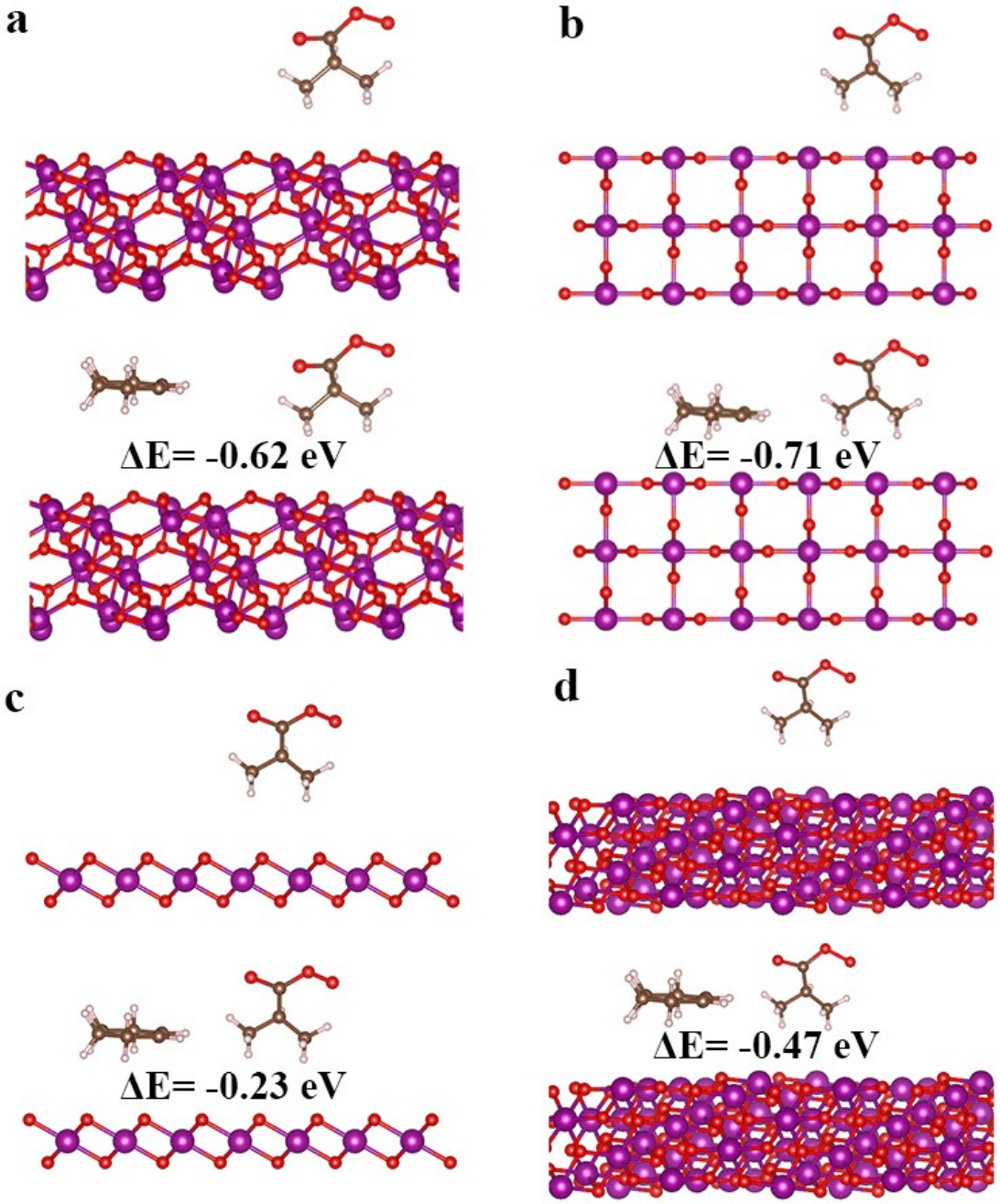

Fig. S5 DFT calculations for the adsorption of cyclohexene on α-MnO_2 (a), β-MnO_2 (b), δ-MnO_2 (c) and γ-MnO_2 (d) samples

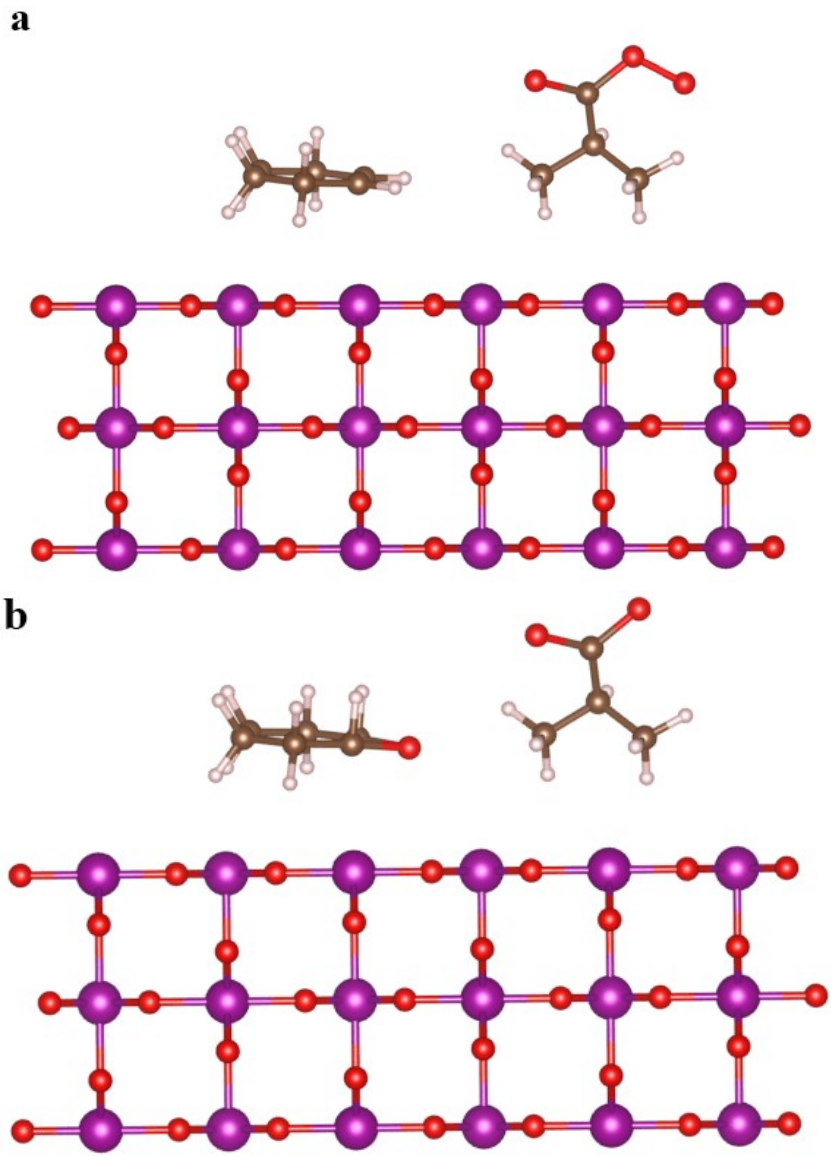

Fig. S6 DFT calculations for the cyclohexene epoxidation reaction on β-MnO_2 heterogeneous catalyst

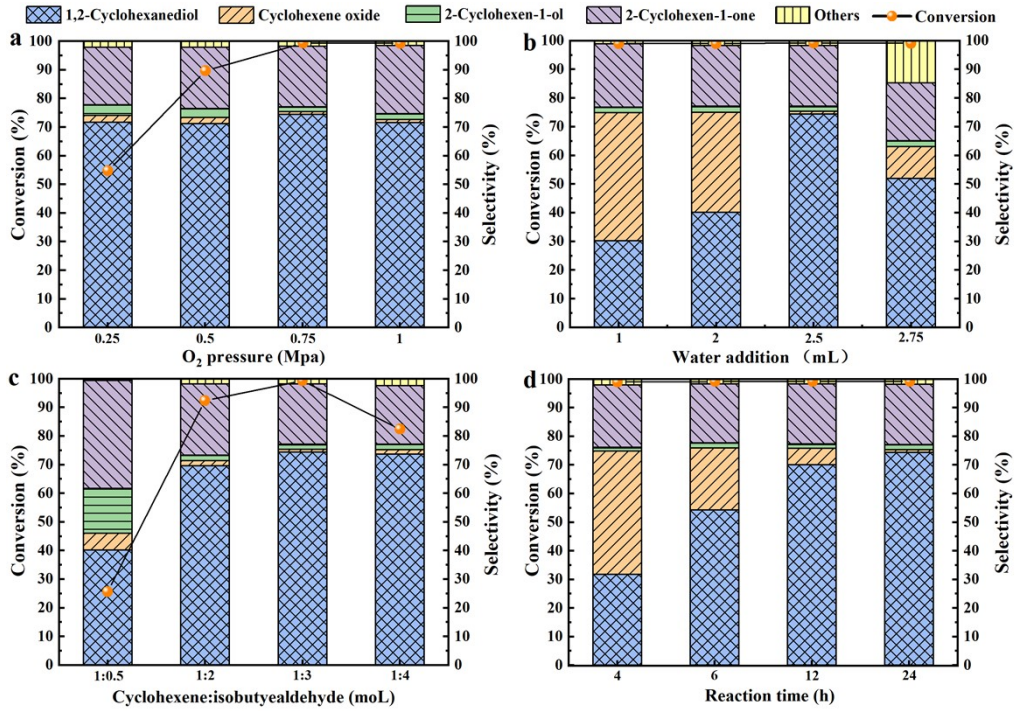

Fig. S7 Influence of O_2 pressure (a), water addition (b), molar ratio of cyclohexene with isobutyraldehyde (c) and reaction time (d) on the cyclohexene conversion and 1,2-cyclohexanediol selectivity

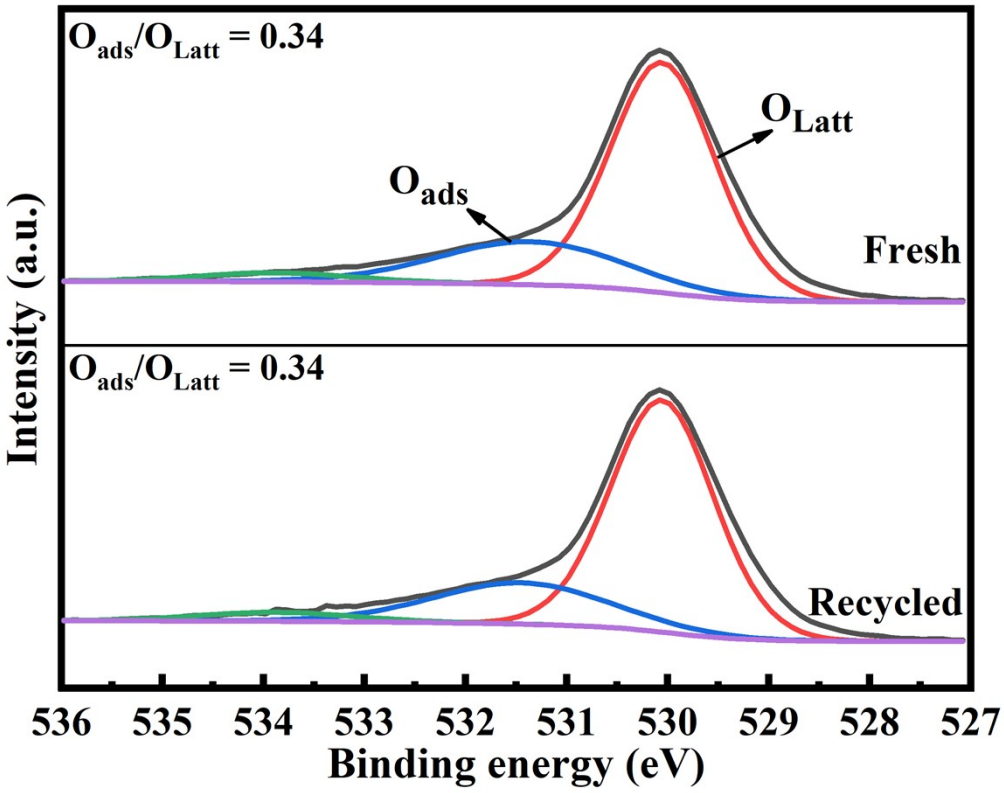

Fig. S8 O1s XPS Spectra of the fresh and recycled β-MnO_2 samples