Supplementary Information

SO_3 decomposition over silica modified β–SiC supported $CuFe_2O_4$ catalyst: Characterization, performance, and atomistic insights

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S.1. Catalyst characterization. Rigaku diffractometer using Ni-filtered with CuK_α radiation at 40 kV and 15 mA was employed to obtain the X–ray diffraction (XRD) patterns. Nicolet iS50 FT–IR was used to collect Fourier transform infra–red spectroscopy (FT–IR) spectra in the range of 400–4000 cm^{-1}. Physical Electronics (PHI 5000 Versa Probe III) with an Al Kα was used for

X-ray photoelectron spectroscopy (XPS). The binding energies referenced to the C 1s peak at 284.6 eV. Belsorp-max II instrument was used to determine the Brunauer–Emmett–Teller (BET) surface area and pore volume. FEI Quanta 200 F was used to record the field emission scanning electron microscope–energy dispersive X–ray spectroscopy (FESEM–EDS) and elemental mapping. FEI Tecnai TF20 was employed to capture the transmission electron microscopy (TEM) and high resolution (HR) TEM images.

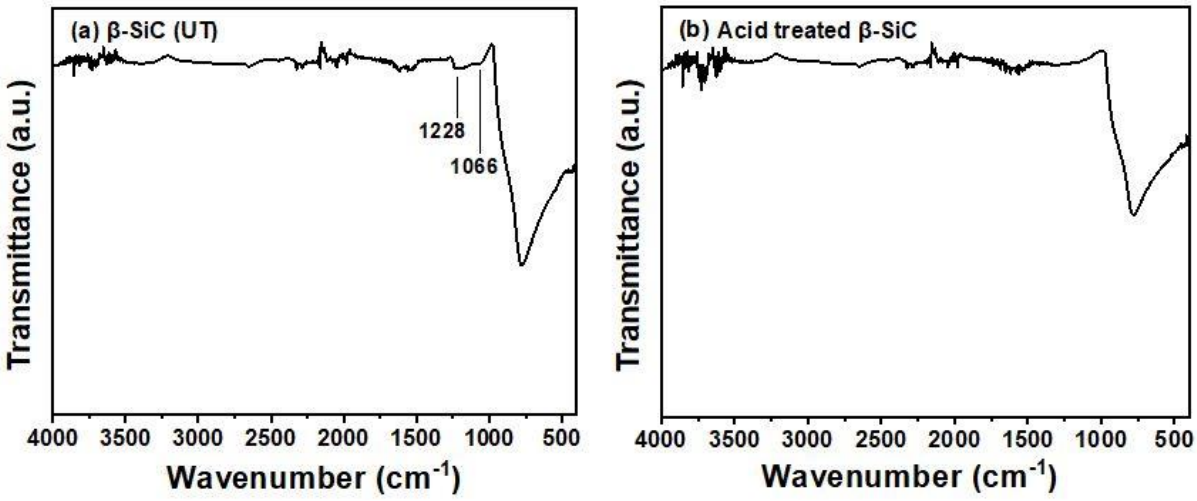

Figure S1 FTIR of (a) β-SiC (UT), and (b) acid treated β-SiC. Acid treatment leads to dissolution of $S_iO_xC_y/SiO_2$ phases and leaving SiC phase which is also evident from the absence of peaks at 1066 to 1164, 1228 cm^{-1} in the FTIR spectra of acid treated β-SiC.

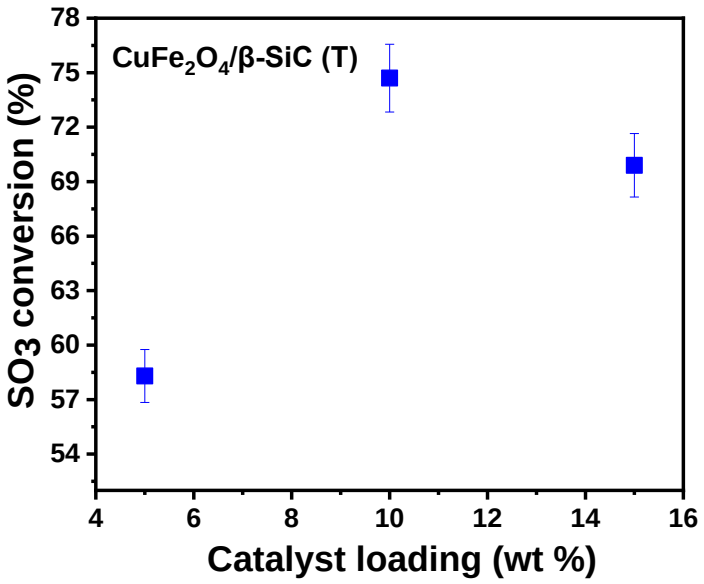

Figure S2 Effect of $CuFe_2O_4$ loading over β-SiC (T) support.

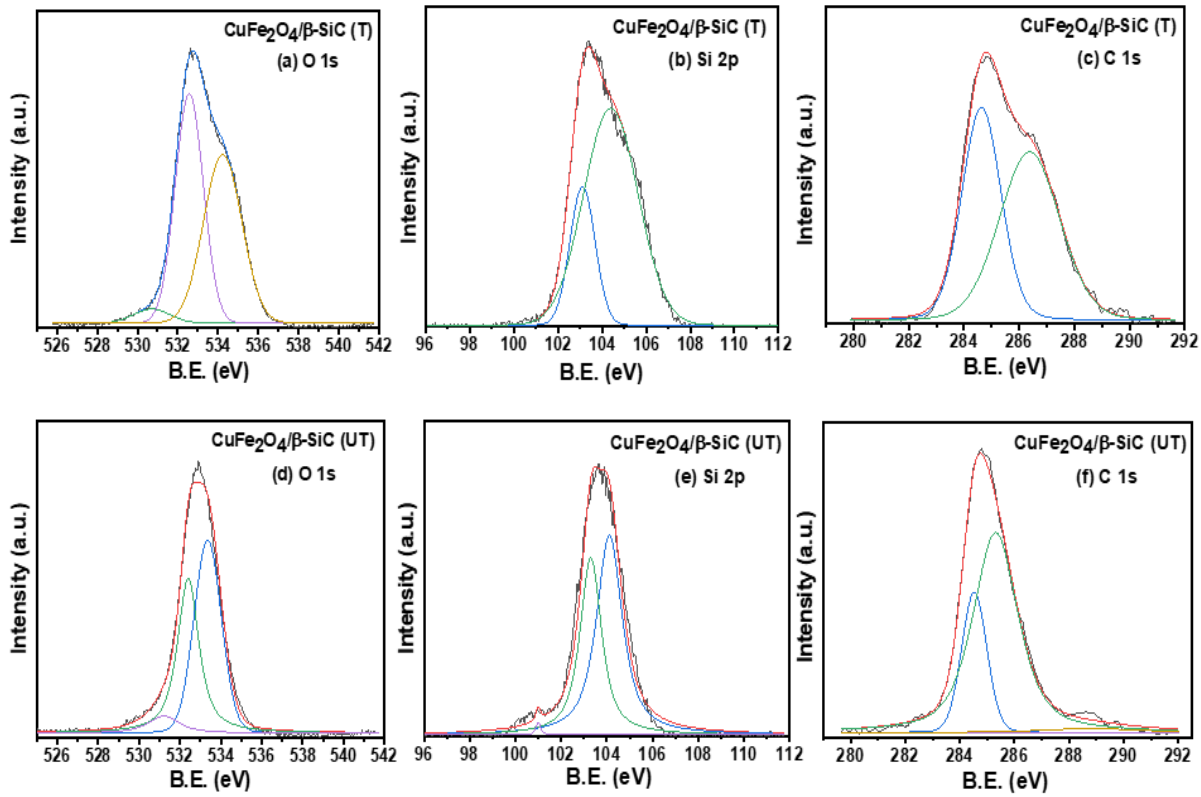

Figure S3 XPS of O 1s, Si 2p, C 1s of the (a–c) $CuFe_2O_4$/β-SiC (T) and (d–f) $CuFe_2O_4$/β-SiC (UT) respectively.

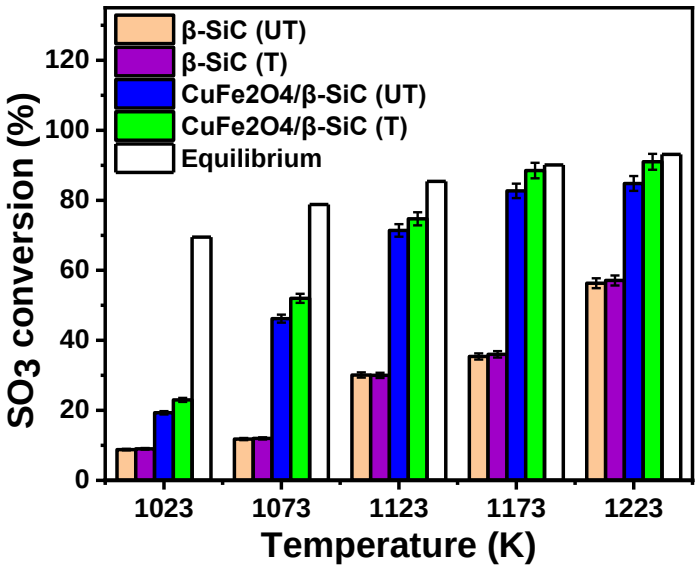

Figure S4 Comparison of SO_3 conversion (%) of β-SiC (UT) and β-SiC (T) with $CuFe_2O_4$/β-SiC (T) and $CuFe_2O_4$/β-SiC (UT) in the temperature range of 1023–1223 K.

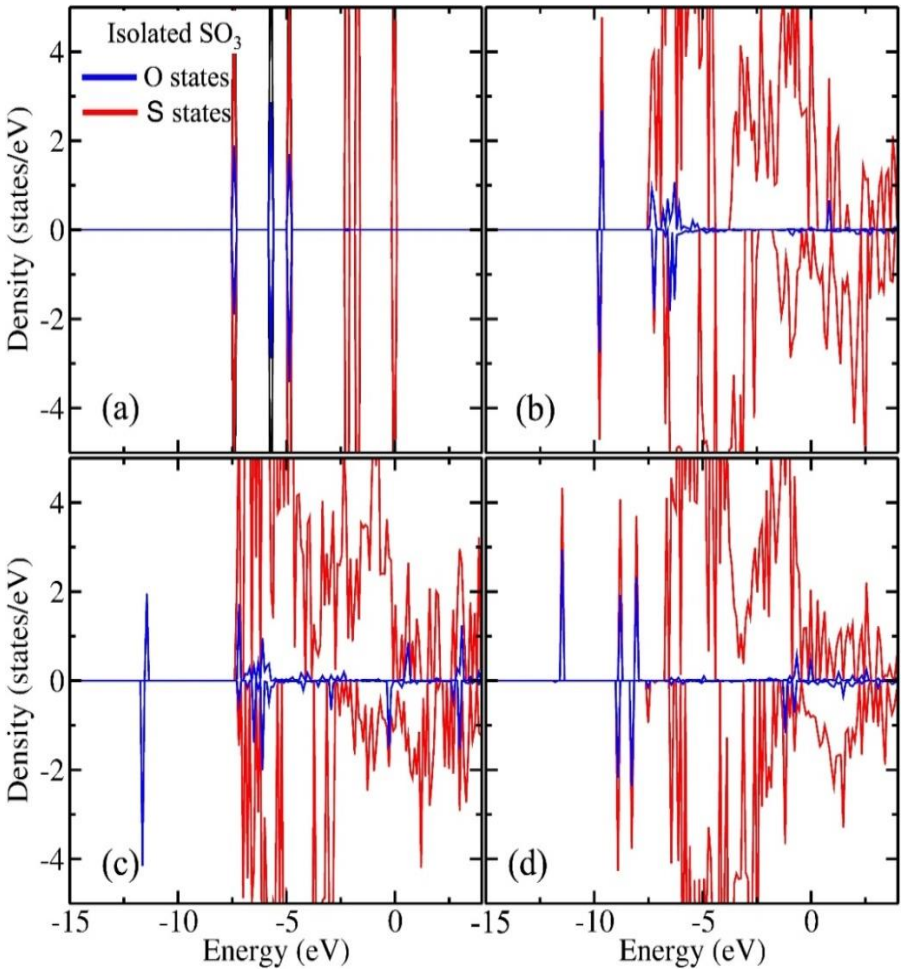

Figure S5 Partial density of states (pDOS) for (a) isolated SO_3, SO_3 adsorbed over the cluster (b) $CuFe_2O_4$, (c) $CuFe_2O_4$ with O-vacancy and (d) Fe_2O_3 with O-vacancy. Here, blue and red colors correspond to S and O states, respectively.