

Supporting information

The charge distribution of atoms on styrene has been calculated by the density functional theory (DFT) method at the B3LYP/ (6-311G (d) level using Gaussian 09 program. The calculated results were as follows:

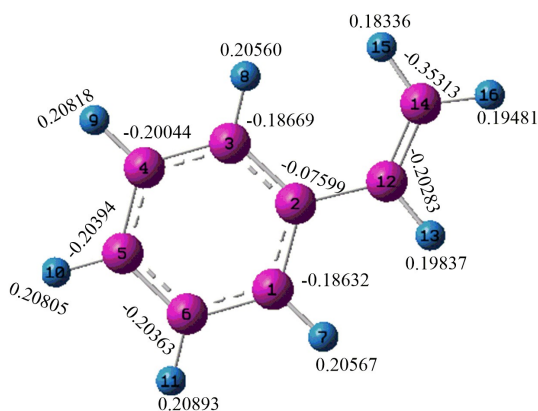


Figure S1 The calculated distribution of NBO charge for styrene

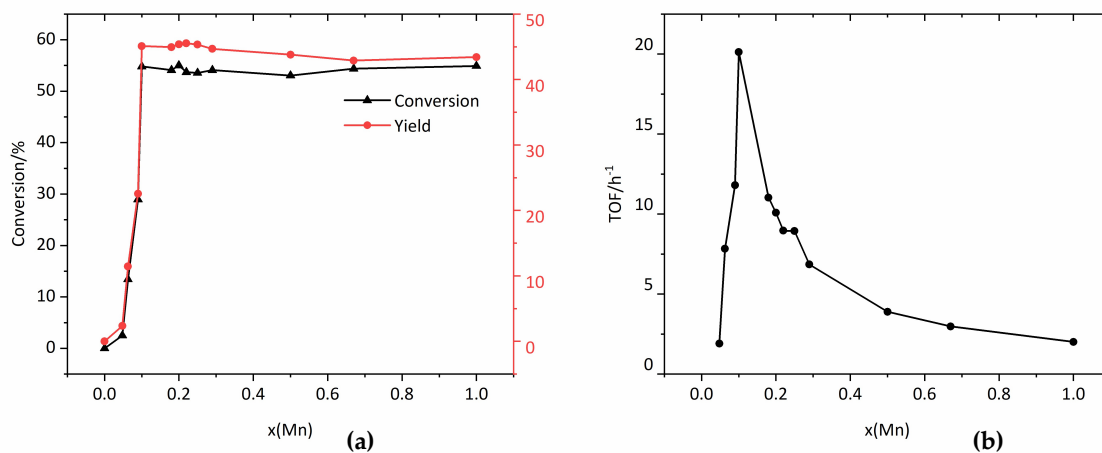


Figure S2. (a) Plots of conversion of styrene and the yield of styrene oxide versus a series of $\text{Mn}_x\text{Cu}_y\text{-MOFs}$, 3h.

(b) The TOF per Mn site with different mole ratio of Mn, 3h.