# Electronic Supplementary information

**Synergistic activation of persulfate by manganese cobalt oxide/reduced graphene oxide nanocomposite with enhanced degradation of trichloroethylene**

Lu Zhang[a, b], Pengfei Ji[a], Rui Song[a], Jiayuan Li[a], Kaifeng Qin[b] and Gang Xu[*a, b]

[a]School of Environmental and Chemical Engineering, Shanghai University, 99 Shangda Road, Shanghai 200444, P.R. China.

[b]Key Laboratory of Organic Compound Pollution Control Engineering, Ministry of Education, Shanghai 200444, P.R. China.

† Gang Xu, E-mail addresses: xugang@shu.edu.cn

**Computational Details.** Density functional theory (DFT) calculations were performed by using the Vienna ab Initio simulation package (VASP). The projector augmented wave (PAW) potentials and generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof (PBE) functional were used for the electron-ion interaction and exchange-correlation energy, respectively. The cutoff energy of the plane wave basis was set to 400 eV. The convergence criteria for the total energy and force were set to $10^{-5}$ eV and 0.02 eV $Å^{-1}$, respectively. The DFT-D3 correction method was used to describe the van der Waals (vdW) interaction. A vacuum distance of at least 15 Å in the z direction was imposed to eliminate the interactions between the periodic images.

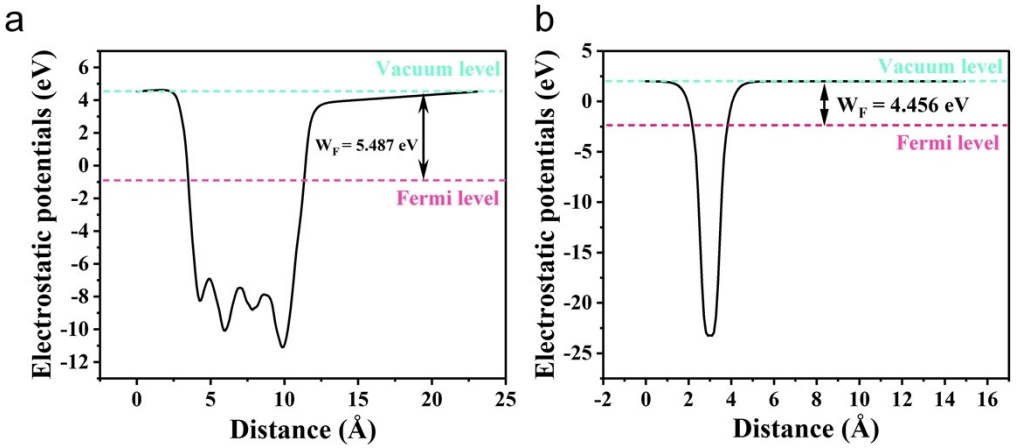


**Fig. S1** Potential diagrams of (a) $MnCo_2O_4$ (311) and (b) rGO surface obtained from first-principles simulations.

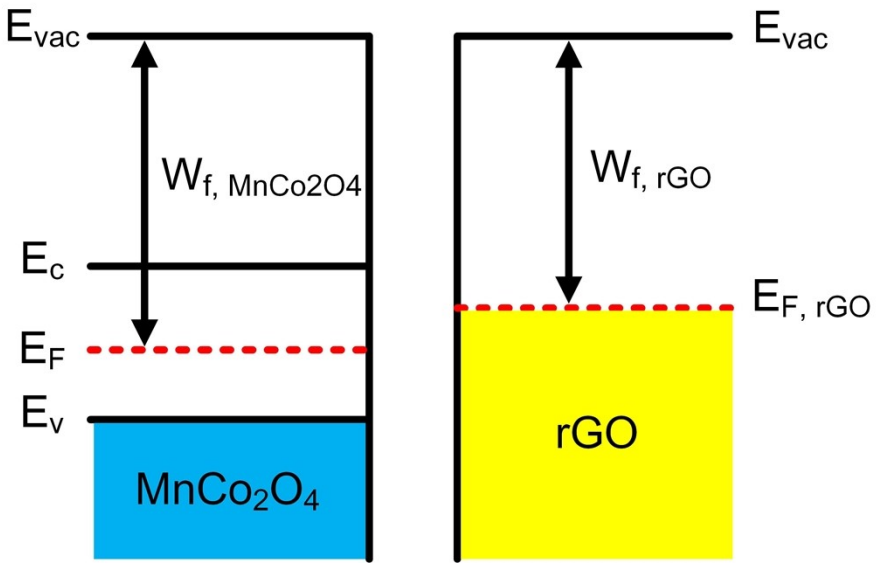


**Fig. S2** Energy band diagrams of $MnCo_2O_4$ and rGO contacts: $E_{vac}$, vacuum energy; E*c*, energy of conduction band minimum; E*v*, energy of valence band maximum; $W_f$, $MnCo_2O_4$, $MnCo_2O_4$ work function; $W_{f,\ rGO}$, rGO work function;

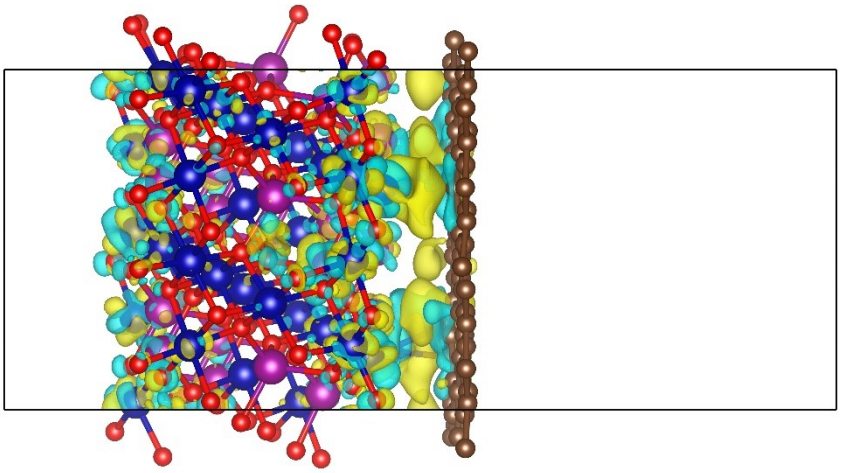

**Fig. S3** Charge density difference of $MnCo_2O_4$ and rGO. The blue, purple, red, and brown represent the elements of cobalt, manganese, oxygen and carbon, respectively.

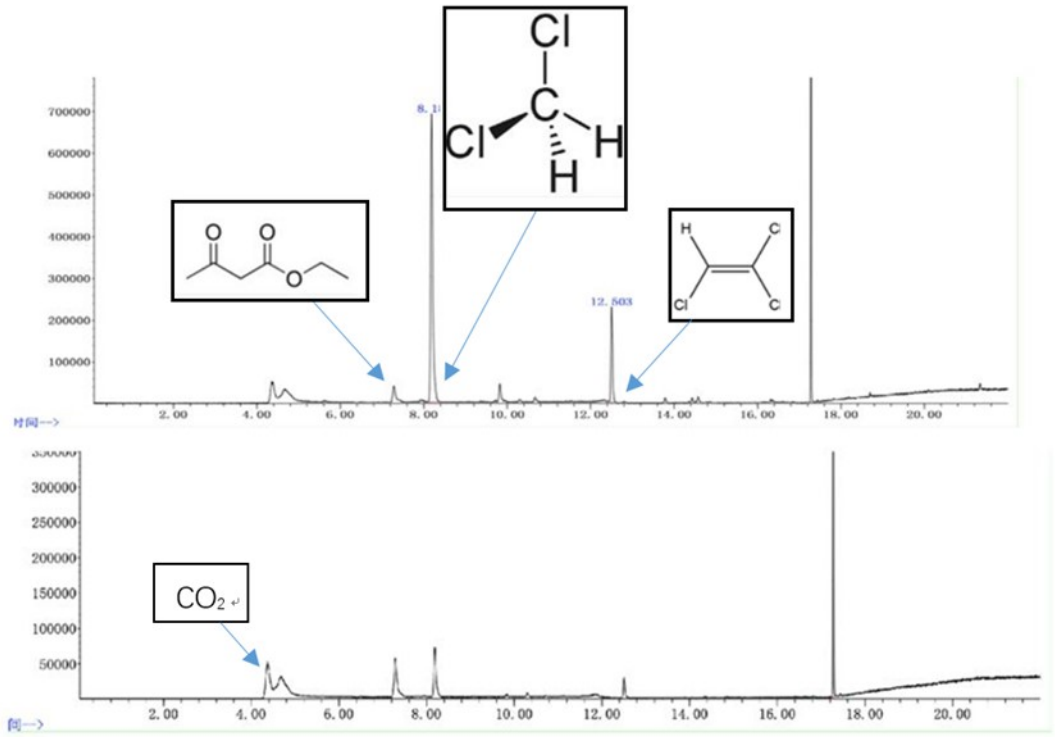


**Fig. S4** The GC-MS spectrum of TCE degradation