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# Synergetic Effect of Calcium Doping on Catalytic Activity of Manganese Ferrite: DFT Study and Oxidation of Hydrocarbon

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## Supporting Information

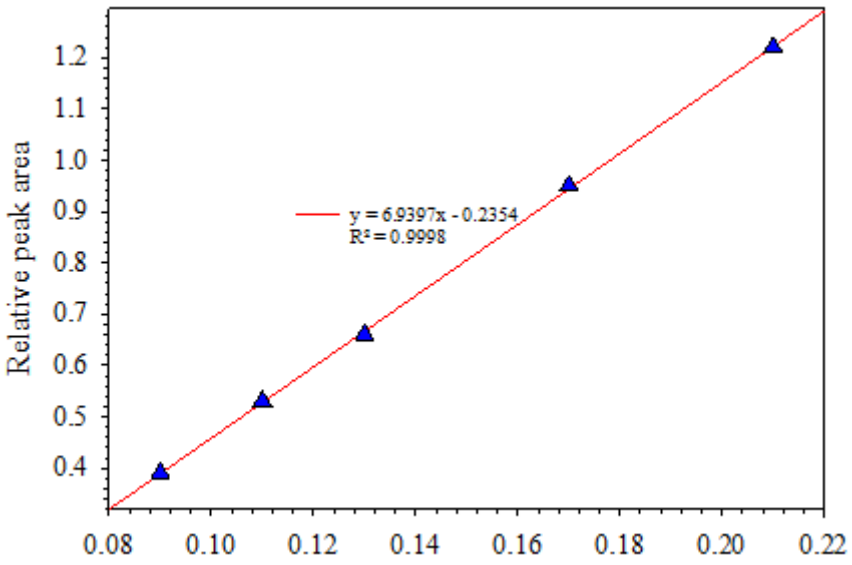


**Figure SI 1.** Calibration curve of CH in a mixture solution of CHOH and RCOR.

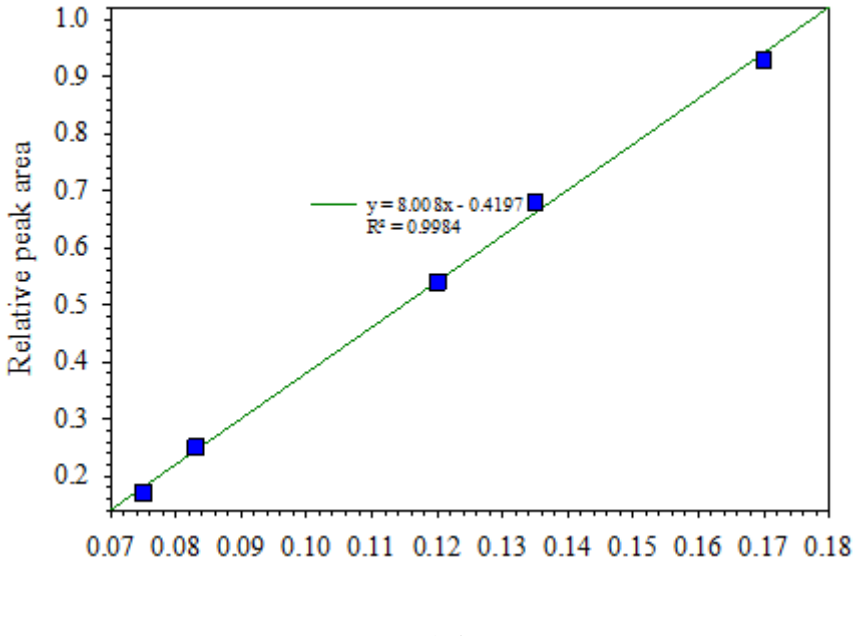


**Figure SI 2.** Calibration curve of COH in a mixture solution of CH and RCOR.

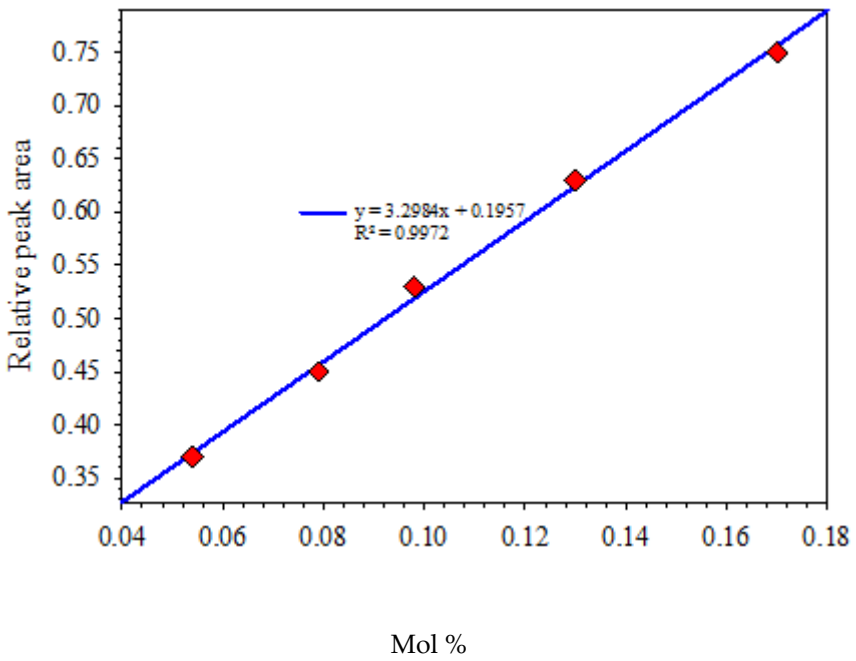


**Figure SI 3.** Calibration curve of RCOR in a mixture solution of CH and COH.

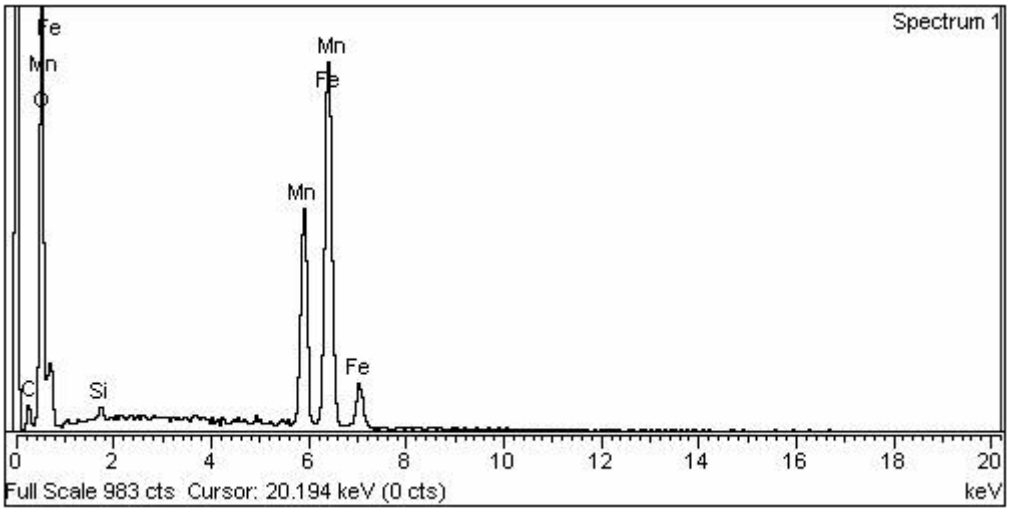


**Figure SI 4.** EDX spectrum of $MnFe_2O_4$.

**Table SI 1.** Magnetic moment for Mn-ferrite and Ca- Mn-ferrite.

| |
|---|
| Undoped:MMINT:MAGNETIC MOMENT IN INTERSTITIAL = 6.20112 |
| Mn = 4.20919 |
| Fe = 3.81705 |
| O = 0.29206 |
| Mnx8 = 33.67352 |
| Fex16= 61.0728 |
| Ox32 = 9.34592 |
| Total Magnetic moment of unit cell =110.29336 |
| Total Magnetic moment of formula unit =13.78667 |
| doped |
| :MMINT: MAGNETIC MOMENT IN INTERSTITIAL = 4.77769 |
| Ca = 0.03714 |
| Mn = 4.20592 |
| Fe = 3.90299 |
| O = 0.29848 |
| Cax4 = 0.14856 |
| Mnx4 = 16.82368 |
| Fex8 = 62.44784 |
| Ox32 = 9.55136 |
| Total Magnetic moment of unit cell = 93.63771 |
| Total Magnetic moment of formula unit = 11.70471375 |