Electronic Supplementary Material (ESI) for Green Chemistry
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Supporting Information

Preparation of $CuCr_2O_4$ Spinel Nanoparticles Catalyst for Selective Oxidation of Toluene to Benzaldehyde in Liquid Phase†

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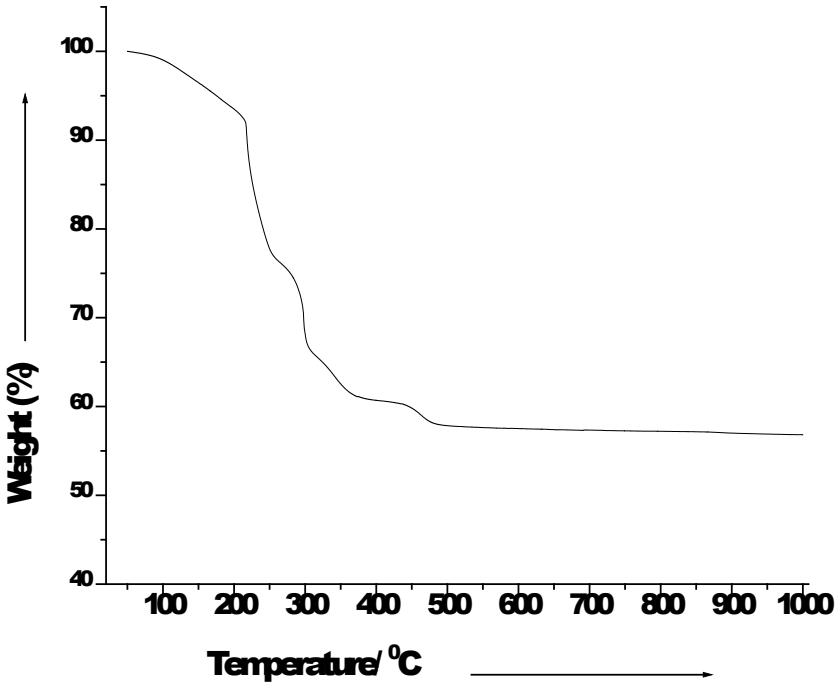

Fig. S1 TGA analysis of uncalcined $CuCr_2O_4$ spinel nanoparticles catalyst.

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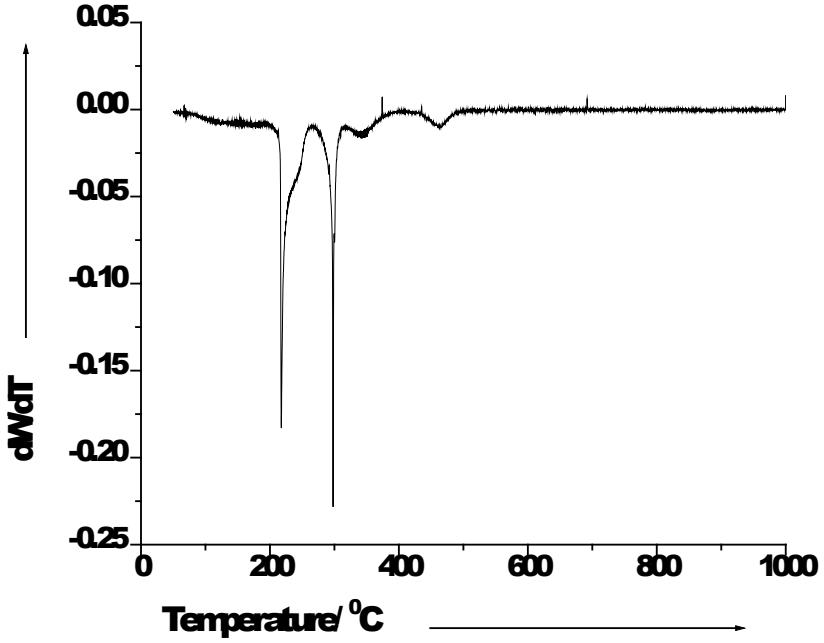

Fig. S2 DTA analysis of the $CuCr_2O_4$ spinel nanoparticles catalyst.

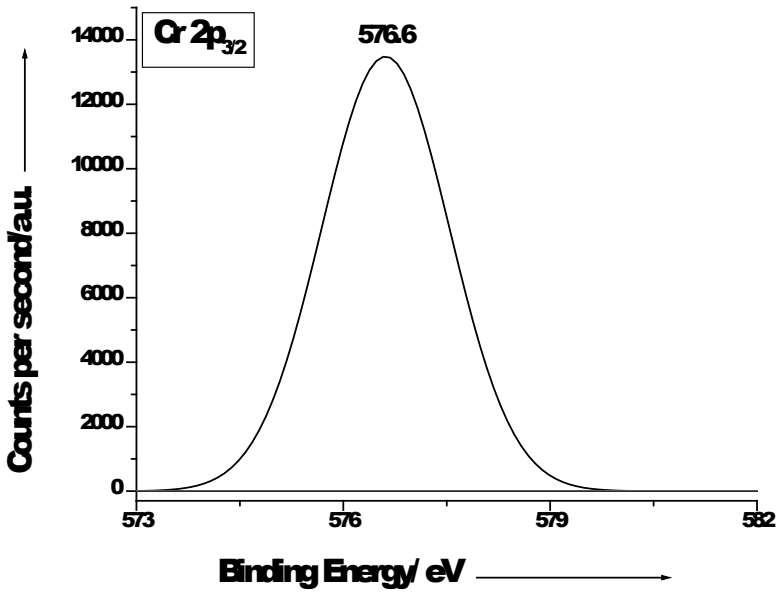

Fig. S3 Cr $2p_{3/2}$ core level spectra of $CuCr_2O_4$ nanoparticles catalyst.

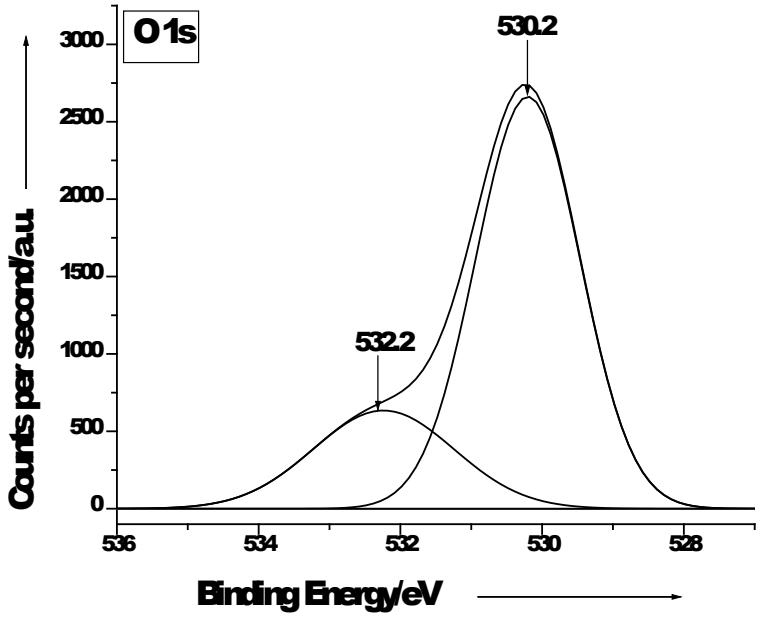

Fig. S4 O_{1s} core level spectra of $CuCr_2O_4$ nano particles catalyst.

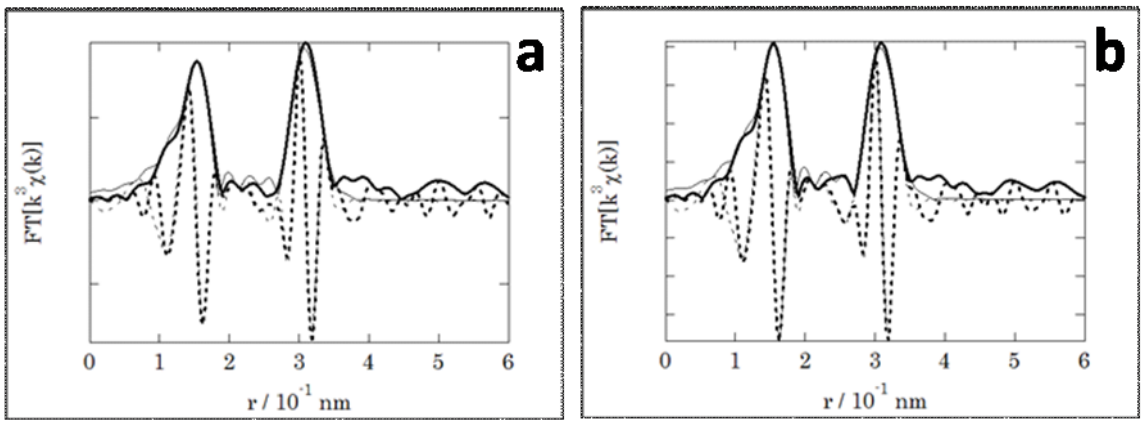

Fig. S5 Fourier Transform of Cu-K edge EXAFS spectra of a) fresh catalyst and b) spent catalyst (after 5 recycle). Amplitude: solid curves; imaginary part: dotted curves; observed data: thick curves; fitting data: thin curves.

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Fresh Catalyst					Spent Catalyst (after 5 recycle)				
No	**Path**	**CN**	**R**	**DW**	**No**	**Path**	**CN**	**R**	**DW**
1	feff0001	4.00	1.886	1.302e-002	**1**	feff0001	4.00	1.885	1.466e-002
2	feff0002	4.00	3.140	1.697e-002	**2**	feff0002	4.00	3.139	1.914e-002
3	feff0003	4.00	3.245	7.268e-003	**3**	feff0003	4.00	3.243	8.193e-003
4	feff0004	8.00	3.370	2.279e-002	**4**	feff0004	8.00	3.369	2.569e-002
5	feff0005	8.00	3.466	7.336e-003	**5**	feff0005	8.00	3.464	8.271e-003
6	feff0006	4.00	3.531	2.436e-002	**6**	feff0006	4.00	3.529	2.746e-002
7	feff0007	4.00	3.545	6.609e-003	**7**	feff0007	4.00	3.543	7.452e-003
8	feff0008	8.00	3.546	1.721e-002	**8**	feff0008	8.00	3.545	1.941e-002
9	feff0009	8.00	3.549	9.517e-003	**9**	feff0009	8.00	3.547	1.073e-002
10	CuO	2.46	1.938	3.646e-003	**10**	CuO	2.52	1.939	3.586e-003

Although, three paths of $CuCr_2O_4$ (feff0001, feff0002, feff0003) crystal were shown in the Table S1but nine paths below 0.36 nm were necessary for fitting. The former Cu-O path can be fitted as 0.1932 – 0.1939 nm that can be attributed to the distance of Cu^{2+} - O of the monatomically dispersed Cu^{2+} species around nanocrystal of $CuCr_2O_4$.

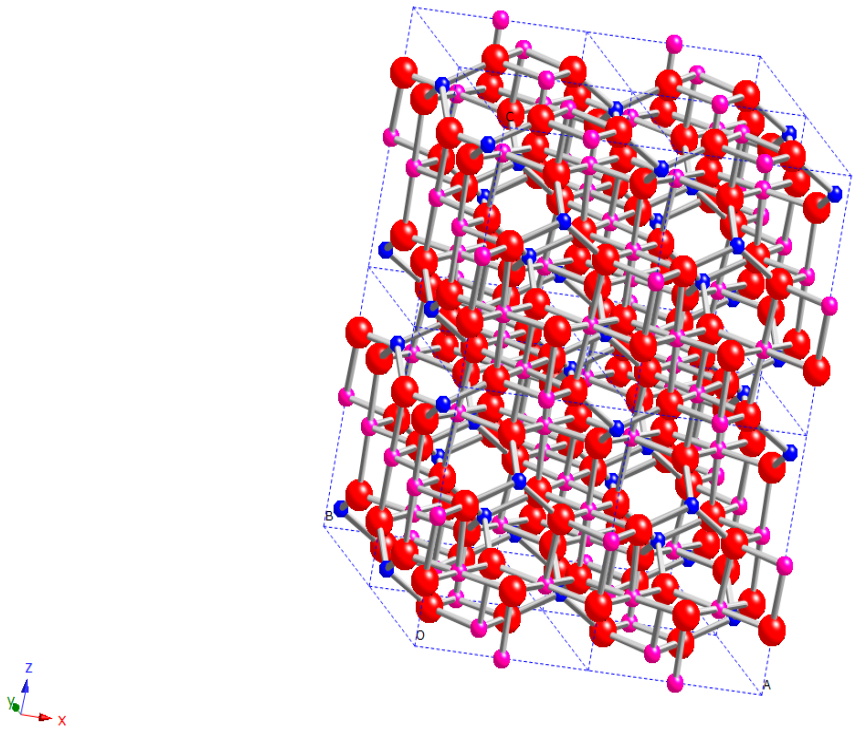
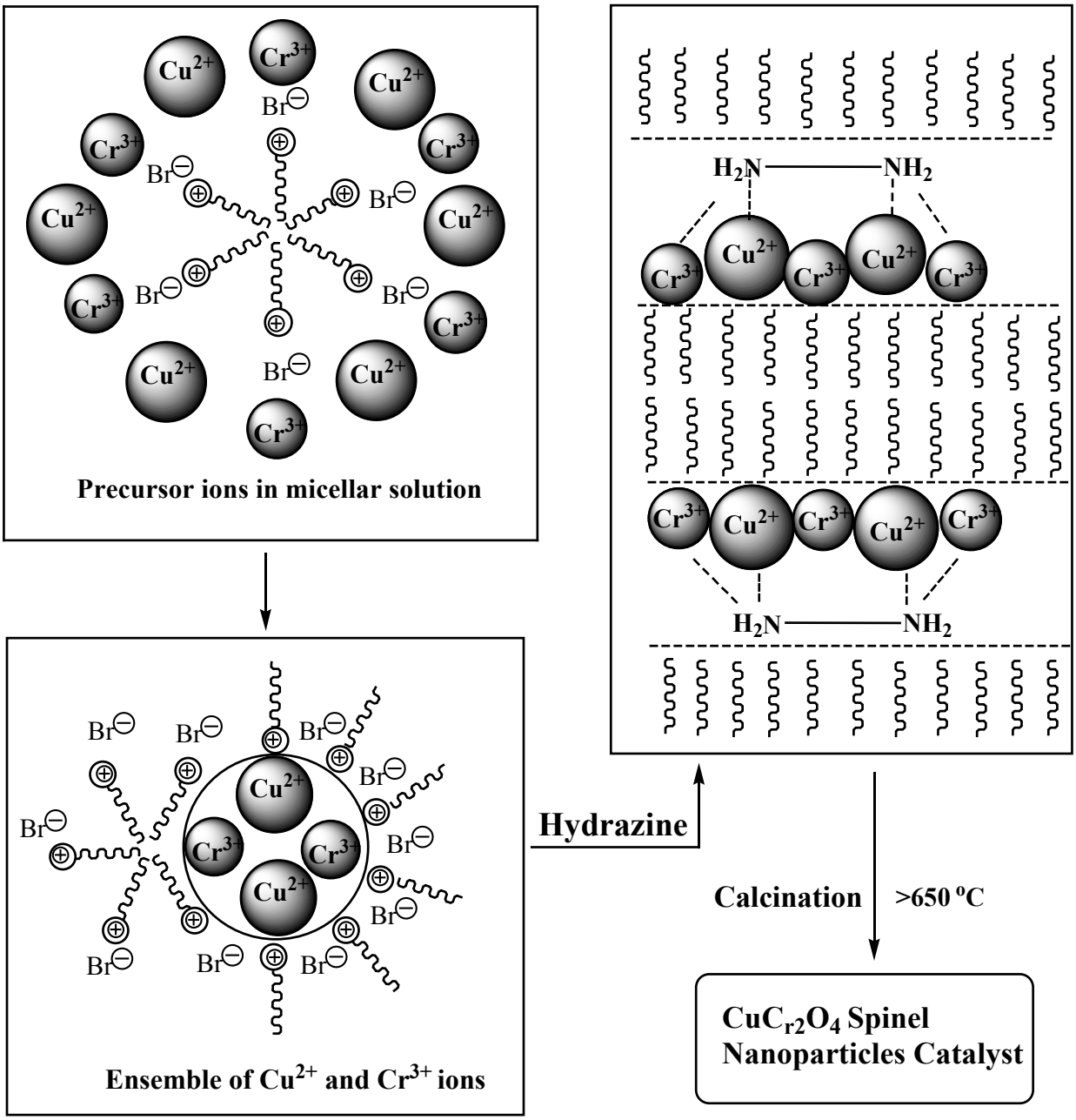


Fig. S6 Model diagram of $CuCr_2O_4$ spinel catalyst: where Cu^{II} occupies 1/8th of the tetrahedral holes and Cr^{III} occupies ½ of the octahedral holes in the ccp array of O^{2-} ions.

Large red balls: O atoms, pink balls: Cr atoms, blue balls: Cu atoms.



Scheme S1 Probable mechanistic way for the generation of $CuCr_2O_4$ spinel NPs

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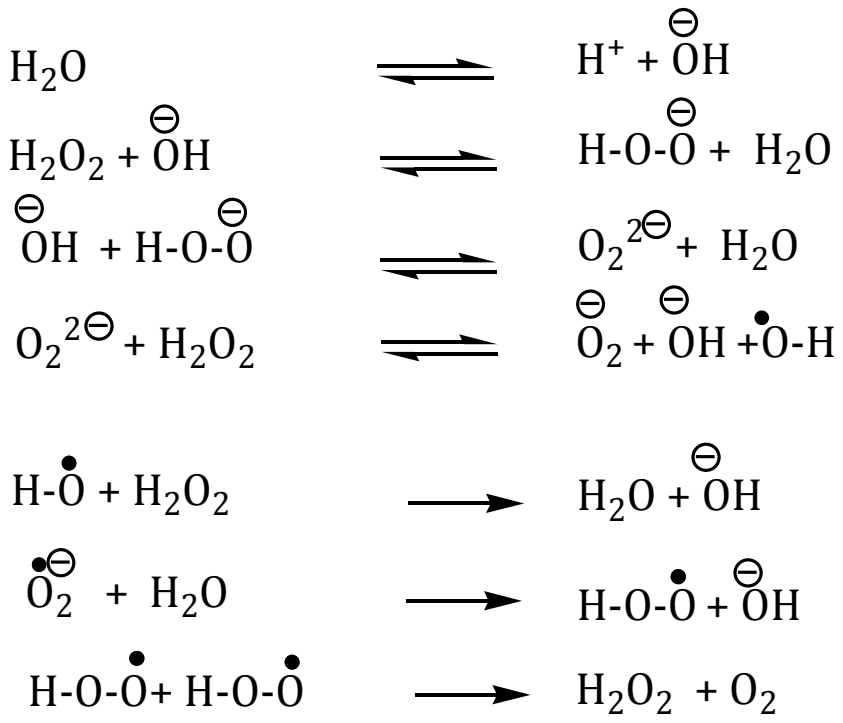
H_2O_2 Dissociation



Scheme S2 Probable mechanistic path for H_2O_2 dissociation.