

SUPPORTING INFORMATION

Vibrational and structural study of environmentally persistent free radicals (EPFRs) formed by phenol dosed metal oxide nanoparticles

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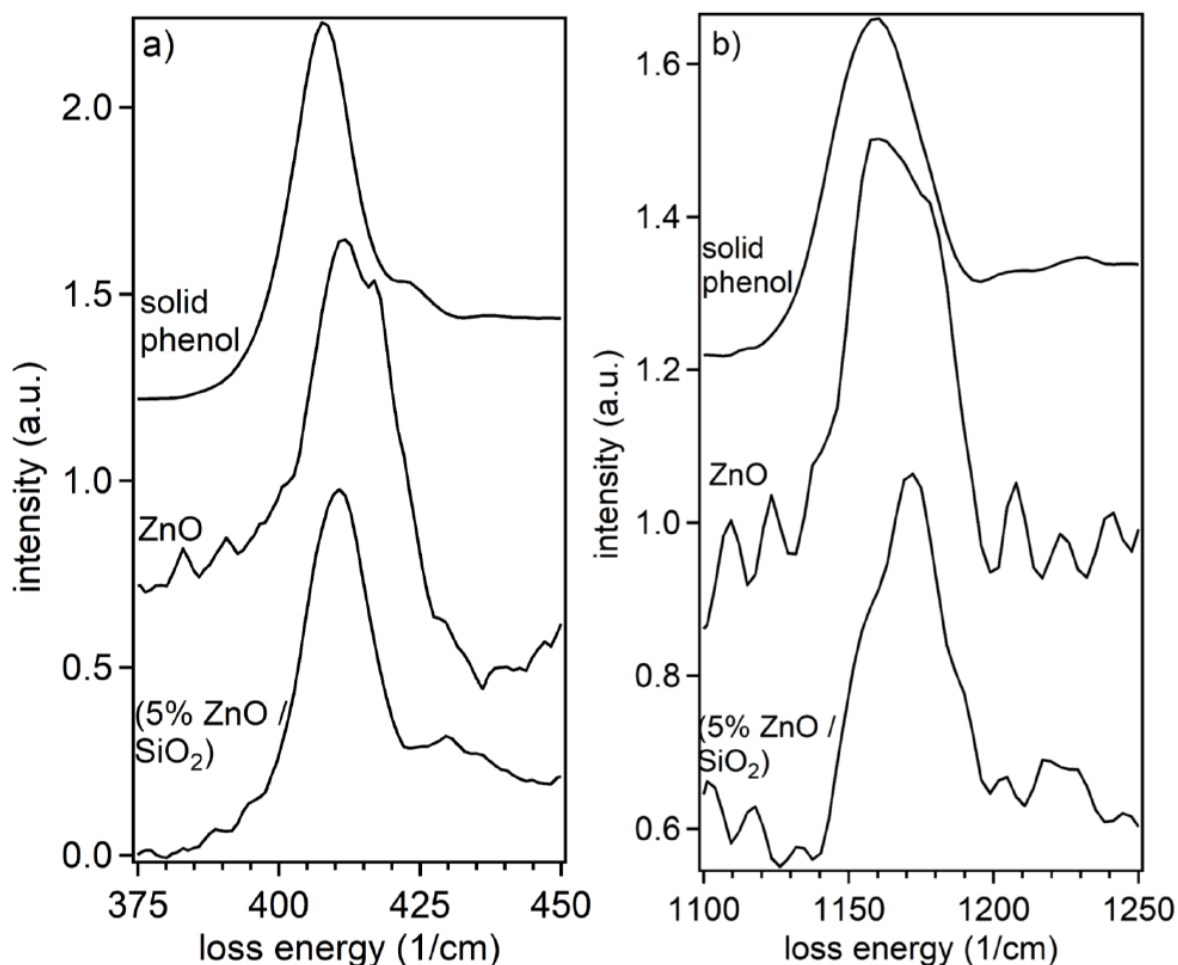


Fig. S1. Inelastic neutron scattering spectra of Zinc oxide powders dosed with phenol at 250°C along with solid phenol reference spectrum (topmost trace). Blank (un-dosed) spectra of powders inside the appropriate sample containers have been subtracted from each of the spectra from the oxides. Figure (a) shows the region containing an out-of-plane bending motion of the phenyl ring, (b) shows a C-H in-plane stretch.

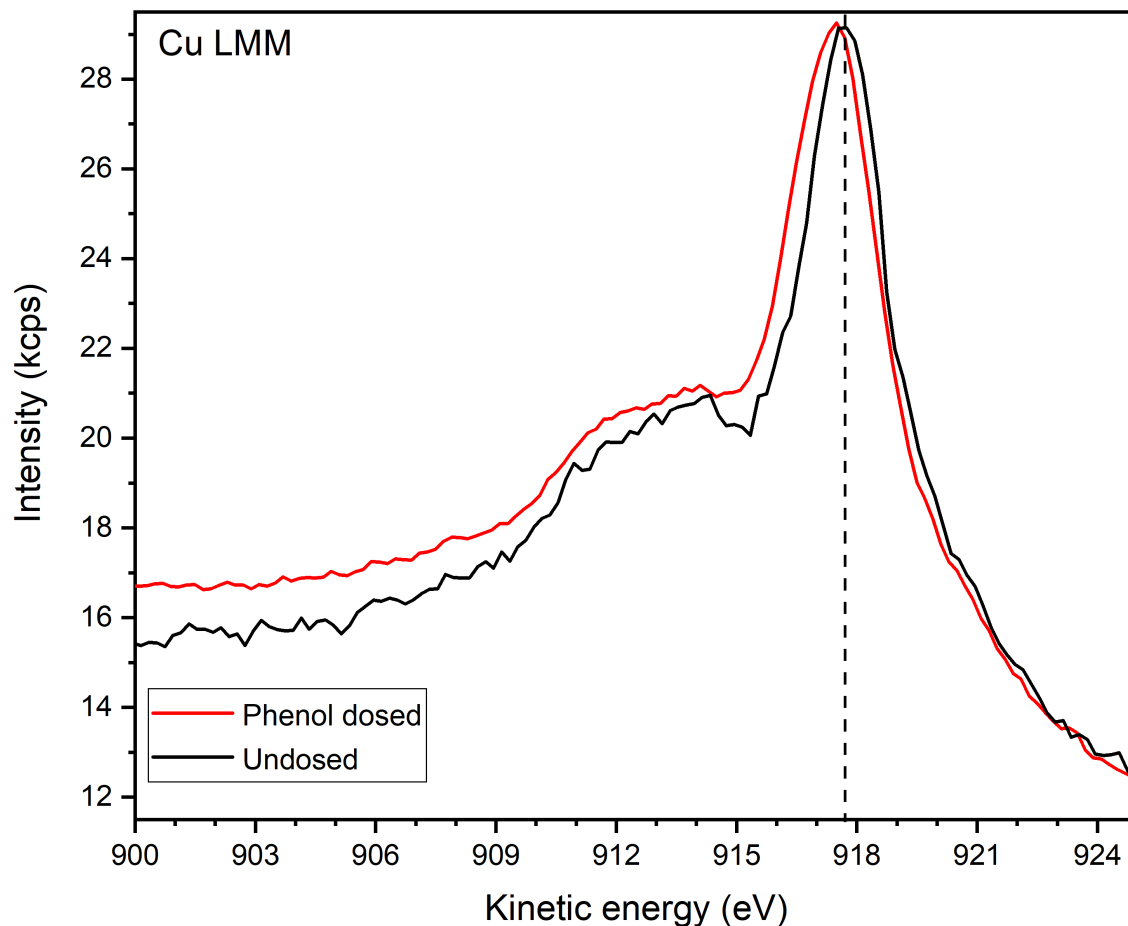


Fig. S1. X-ray photoemission spectrum of Cu LMM transition of undosed (black) and phenol dosed at 250 °C (red) of CuO nanoparticle pellet.

The modified Auger parameter of the dosed surface falls between the reported values¹ for CuO (1851.5 ± 0.4 eV) and Cu₂O (1849.2 ± 0.3 eV), which confirms the partial reduction of Cu²⁺ states.

| | Cu 2p _{3/2} (eV) | Cu LMM (eV) | Modified Auger parameter (eV) |
|------------------------|---------------------------|--------------------|-------------------------------|
| Undosed surface | 933.77 ± 0.0046 | 917.72 ± 0.016 | 1851.49 ± 0.017 |
| Dosed surface | 932.35 ± 0.0017 | 917.49 ± 0.012 | 1849.84 ± 0.012 |

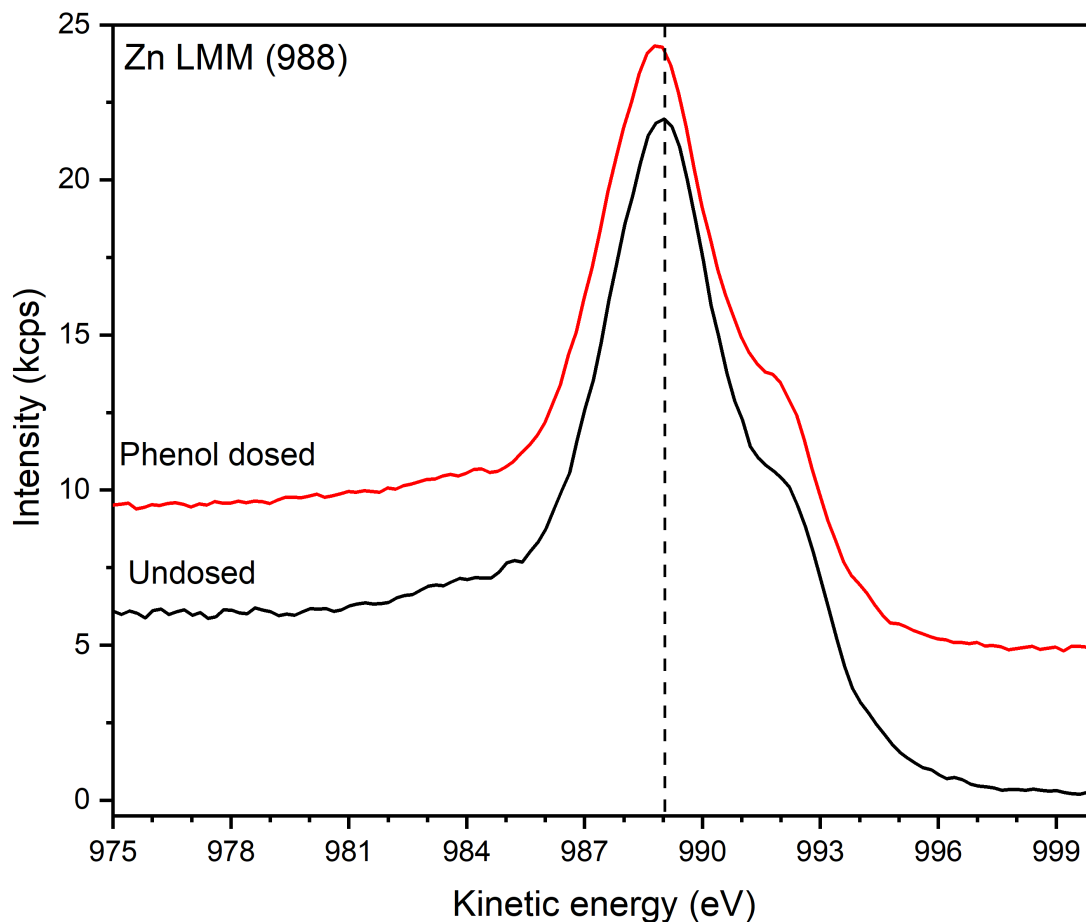


Fig. S2. X-ray photoemission spectrum of Zn LMM (988) transition of undosed (black) and phenol dosed at 250 °C (red) of ZnO nanoparticle pellet.

Zn LMM (988) for:

Undosed surface: 989.04 ± 0.007 eV

Phenol dosed surface: 988.9 ± 0.006 eV

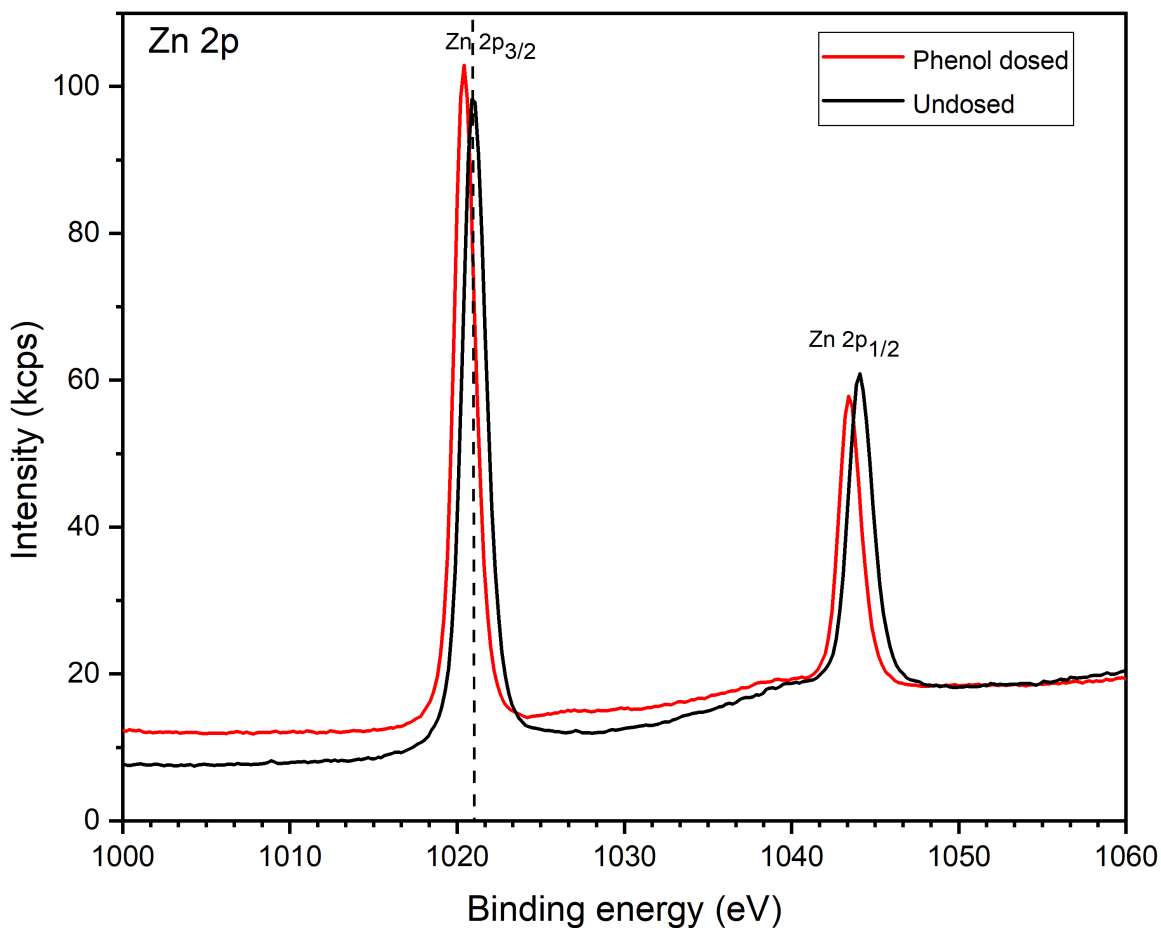


Fig. S3. X-ray photoemission spectrum of Zn 2p region of undosed (black) and phenol dosed at 250 °C (red) of ZnO nanoparticle pellet.

Zn 2p_{3/2} for:

Undosed surface: 1021.01 ± 0.0007 eV

Phenol dosed surface: 1020.4 ± 0.0009 eV

References:

- [1] Wagner, C. D.; Naumkin, A. V.; Kraut-Vass, A.; Allison, J. W.; Powell, C. J.; Rumble, J. R. Jr. NIST Standard Reference Database 20, Version 3.4 (web version) (<http://srdata.nist.gov/xps/>) 2003.