

Electronic Supplementary information (ESI)

ESI-1: EXAFS analysis of nitrogen doped ZnO materials at Zn K edge.

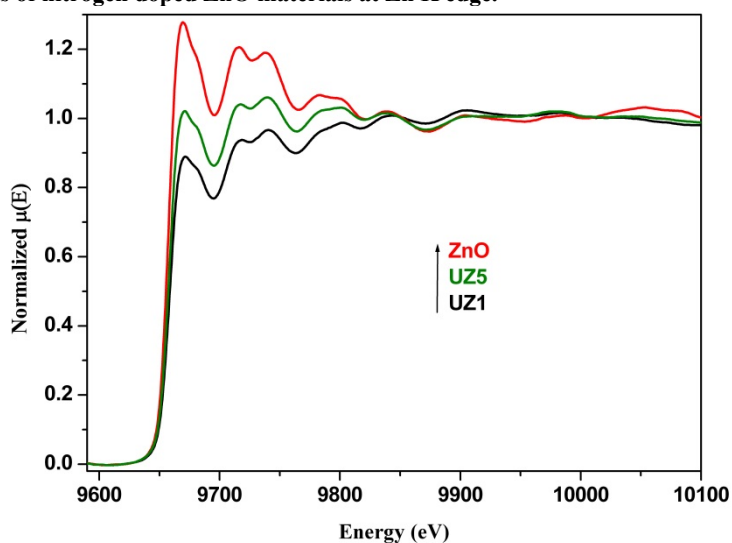


Fig. ESI-1 Normalized EXAFS spectra nitrogen doped ZnO samples measured at Zn K edge along with ZnO as reference. Normalized EXAFS spectra for nitrogen doped ZnO samples are measured at Zn K edge along with bulk ZnO as reference and the corresponding result is given in fig. 1. The edge of lattice Zn shows +2 oxidation state and wurtzite structure as similar that of bulk ZnO.

ESI-2: Analysis of local structural parameters.

Table-ESI-1: Local structural parameters for ZnO_{1-x}N_x (ZU series) evaluated by EXAFS measurements at Zn K edge.

Path	Parameter	ZnO bulk	ZU5 (N=8.6%)	ZU1 (N=15.1%)
Zn-O	R (Å)	1.98	1.95	1.93
	N	4	4	3.68
	σ^2		0.009	0.009
Zn-Zn	R (Å)	3.20	3.12	3.09
	N (6)	6	6	6
	σ^2		0.011	0.009
Zn-Zn	R (Å)	3.25	3.21	3.20
	N		5.4	6.6
	σ^2		0.006	0.005

Nitrogen incorporation is accompanied with growing zinc oxo clusters at the expense of oxygen vacancies. Therefore, bond length parameters are varied with the introduction of N retaining the lattice structure. The bond length of Zn-O decreases with the introduction of nitrogen because of the fact of expected lattice contraction.