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Impact of alkaline metal ions Mg^{2+}, Ca^{2+}, Sr^{2+} and Ba^{2+} on the structural, optical , thermal and antibacterial properties of ZnO nanoparticles prepared by co-precipitation method

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Characterization

X-Ray powder diffraction (XRD) studies

The XRD patterns of the ZnO NPs samples were collected using a X'PERT PRO PANalytical X-ray diffractometer with CuKα (40 kV, 30 mA) radiation source. The ZnO NPs samples were gently crushed before being smeared on a clean glass slide. The powder diffraction patterns were collected over the 2θ in the range between 10˚-80˚ with a scan speed and sampling width of 2 min^{-1} and 0.05˚respectively.

X-ray Photoelectron spectroscopy (XPS) studies

The XPS measurements were performed with XPS instrument (Carl Zeiss) equipped with Ultra 55 FESEM with EDS. All the spectra were acquired at a pressure using ultra high vacuum with Al Kα excitation at 250W.

High Resolution Scanning Electron Microscope studies

HRSEM was performed on the ZnO samples using a FEI - QUANDA 200F microscope operating at 30 kV. The microscope was equipped with a charge-coupled device (CCD) camera. The samples were prepared by 1mg of ZnO NPs samples coated with 1.2 nm gold particle separation on a carbon tape using the low vacuum.

Energy dispersive X-ray spectroscopy studies

Energy dispersive X-ray spectroscopy was done using an EDAX (model: AMETEK) with FEI - QUANDA 200F high resolution scanning electron microscope operated at 30 kV. Dry powdered samples were attached to the substrate using a double-sided carbon tape and mounted onto the sample holder.

Fourier Transforms Infra-Red (FT-IR) spectroscopy studies

Perkin-Elmer Fourier transform infra-red (FT-IR) spectrometer was used in transmission mode and the corresponding spectra were recorded in the range of 4000-400 cm^{-1} using the KBr pellet technique for pure ZnO and alkaline metal ions Mg^{2+}, Ca^{2+}, Sr^{2+} and Ba^{2+} doped ZnO NPs samples .

Photoluminescence (PL) studies

Room temperature PL measurements were performed for the pure ZnO and alkaline metal ions Mg^{2+}, Ca^{2+}, Sr^{2+} and Ba^{2+} doped ZnO NPs samples with excitation wavelength of 254 nm using Jobin yvon Flurolog-3-11 spectrofluorometer having Xenon lamp 450W as a source and resolution of 0.2 nm. The emission spectra were recorded in the UV and visible range (270-600nm) using as software DATA MAX / GRAMS/31.

Thermal analysis

The thermogravimetric and differential thermal analysis was carried out by using of TGA Q500 U20.10 Build 36 thermal analyzer for pure ZnO and alkaline metal ions Mg^{2+}, Ca^{2+}, Sr^{2+} and Ba^{2+} doped ZnO NPs samples recorded in the temperature range 30-800˚C, in nitrogen atmosphere with a heating rate of 20 ˚C min^{-1}.

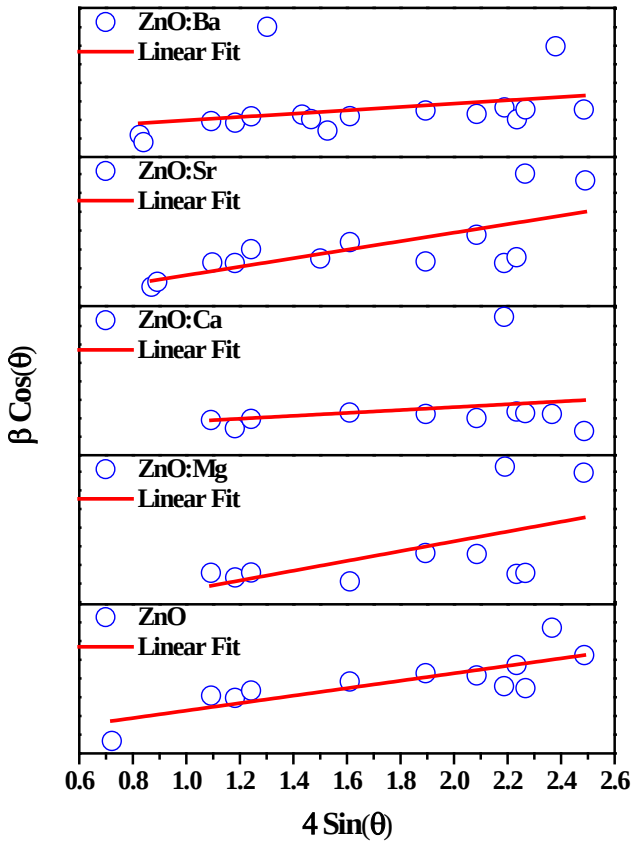

Figure S1. The William-Hall plot analysis of (a) Pure ZnO, (b) ZnO:Mg, (c) ZnO:Ca, (d) ZnO:Sr and (e) ZnO:Ba NPs solid line show the theoretical fit.

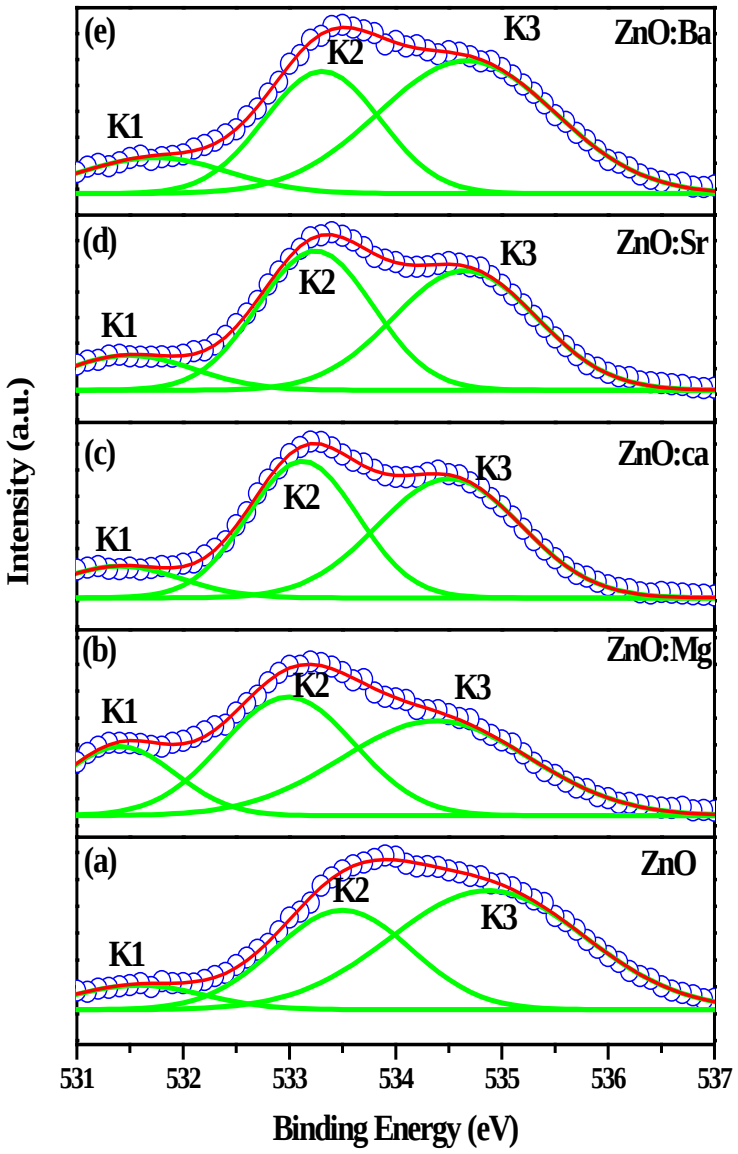

Figure S2. XPS spectra of O (1s) for (a) Pure ZnO, (b) ZnO:Mg, (c) ZnO:Ca, (d) ZnO:Sr and (e) ZnO:Ba NPs.

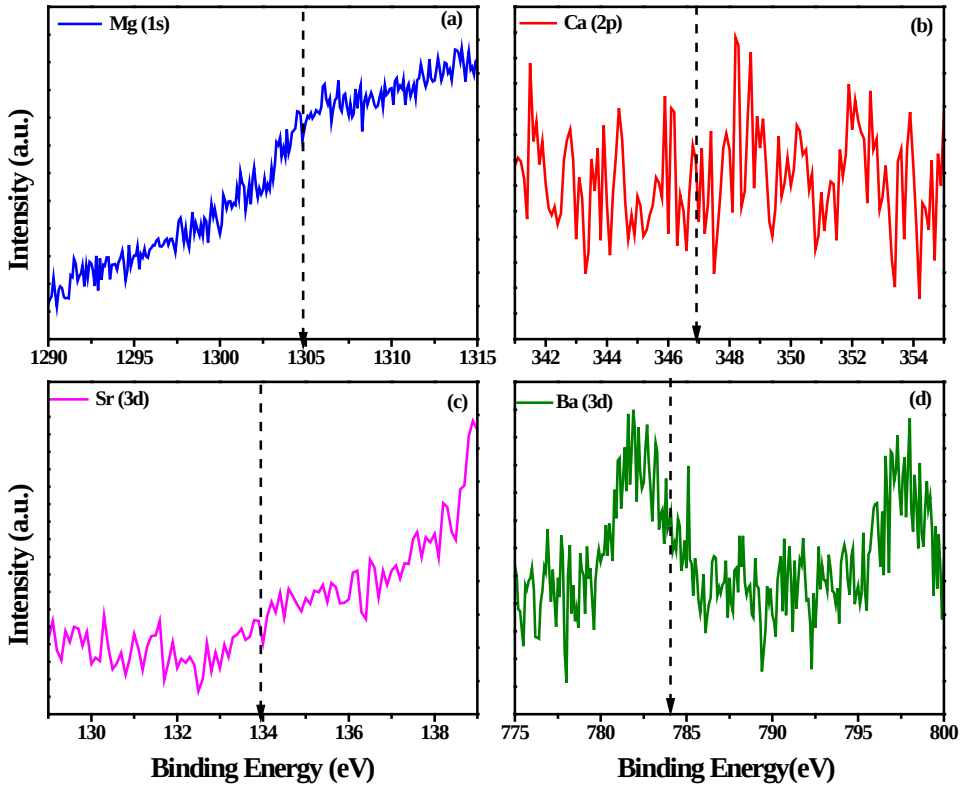

Figure S3. XPS spectra of (a) ZnO:Mg, (b) ZnO:Ca, (c) ZnO:Sr and (d) ZnO:Ba NPs.

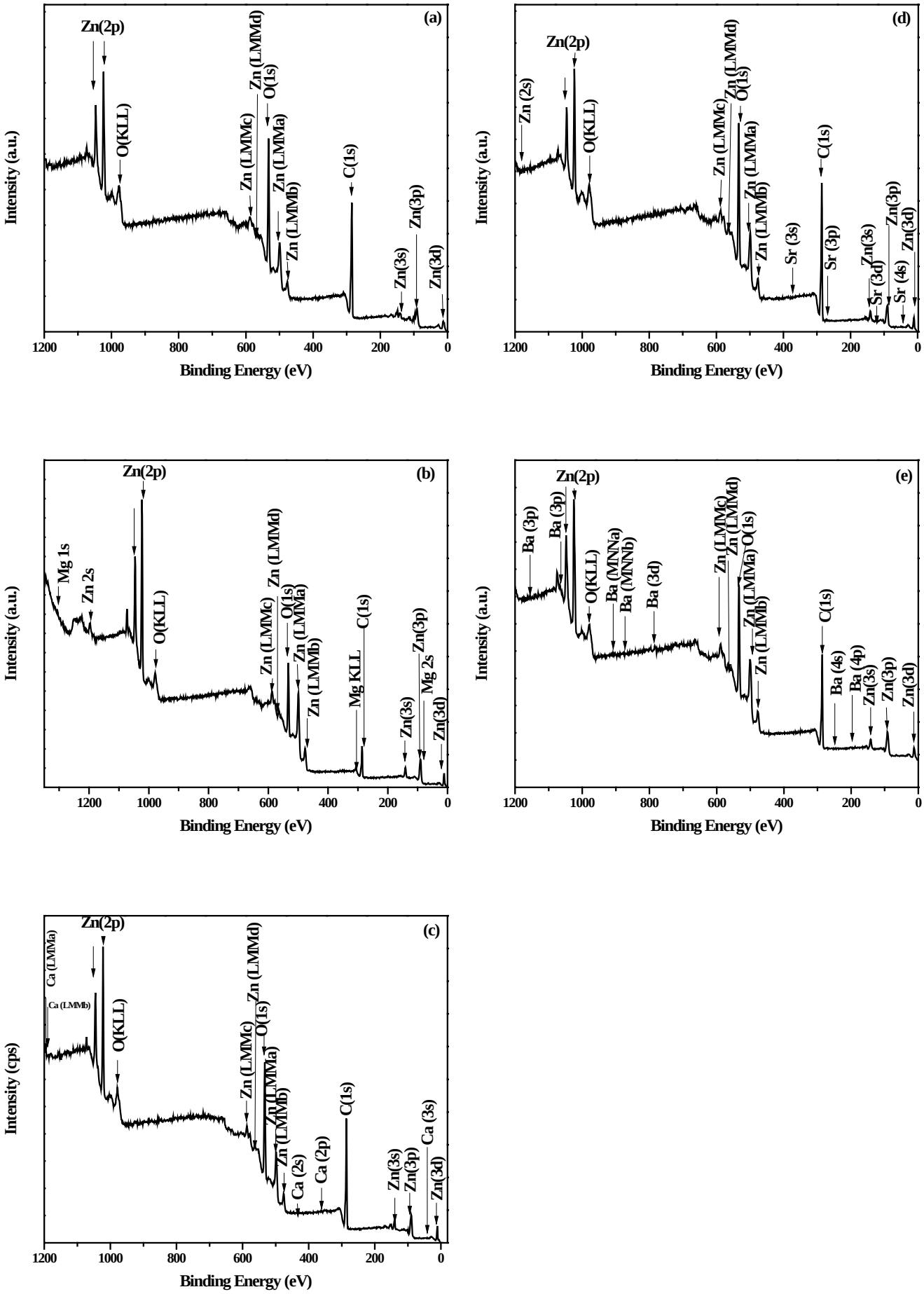

Figure S4. XPS wide scan graph of (a) Pure ZnO, (b) ZnO:Mg, (c) ZnO:Ca, (d) ZnO:Sr and (e) ZnO:Ba.

Table S1. Atomic and Mass Concentration percentage of Pure ZnO and alkaline metal ions doped ZnO NPs for XPS spectra.

Zn 2p		O 1s		Doping %	
Atom. Con%	Mass. Con%	Atom. Con%	Mass. Con%	Atom. Con%	Mass. Con%
18.39	47.94	81.61	52.06	-	-
32.61	66.37	67.15	33.44	0.24 (Mg 1s)	0.18(Mg 1s)
19.29	49.37	80.62	50.48	0.09 (Ca 2p)	0.15(Ca 2p)
16.83	45.22	83.13	54.64	0.04(Sr 3d)	0.14 (Sr 3d)
21.03	51.08	78.53	46.67	0.44 (Ba 3d)	2.25 (Ba 3d)

Table S2. The elemental composition of the synthesized ZnO NPs.

Sample	At%			
	Zn	O	Doping amount	Total
ZnO	61.27	38.73	-	100%
ZnO:Mg	61.79	34.61	3.6(Mg)	100%
ZnO:Ca	53.19	44.64	2.17(Ca)	100%
ZnO:Sr	51.79	46.9	1.31(Sr)	100%
ZnO:Ba	44.72	53.74	1.54(Ba)	100%

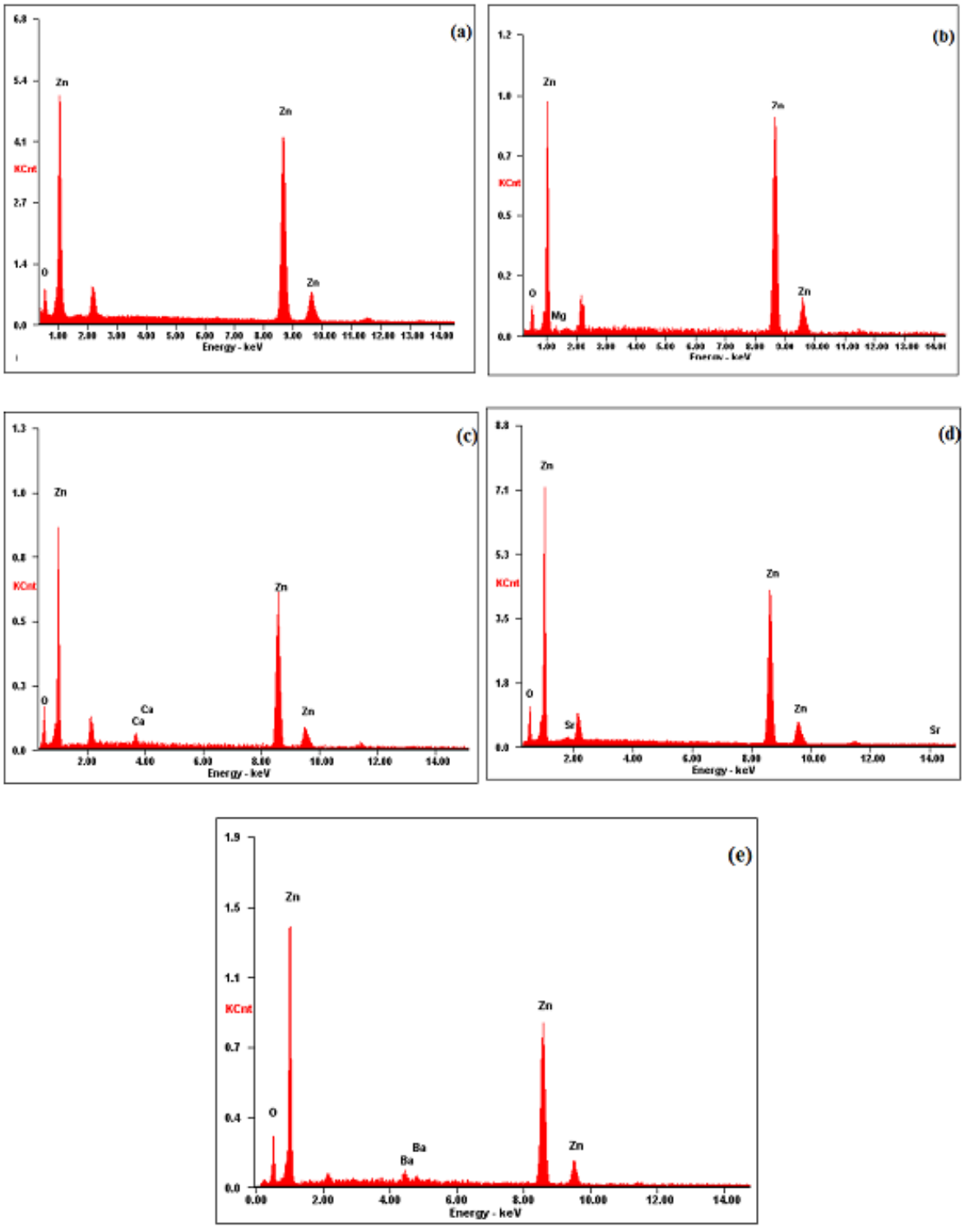

Figure S5. EDAX spectra of (a) Pure ZnO, (b) ZnO:Mg, (c) ZnO:Ca, (d) ZnO:Sr and (e) ZnO:Ba NPs.

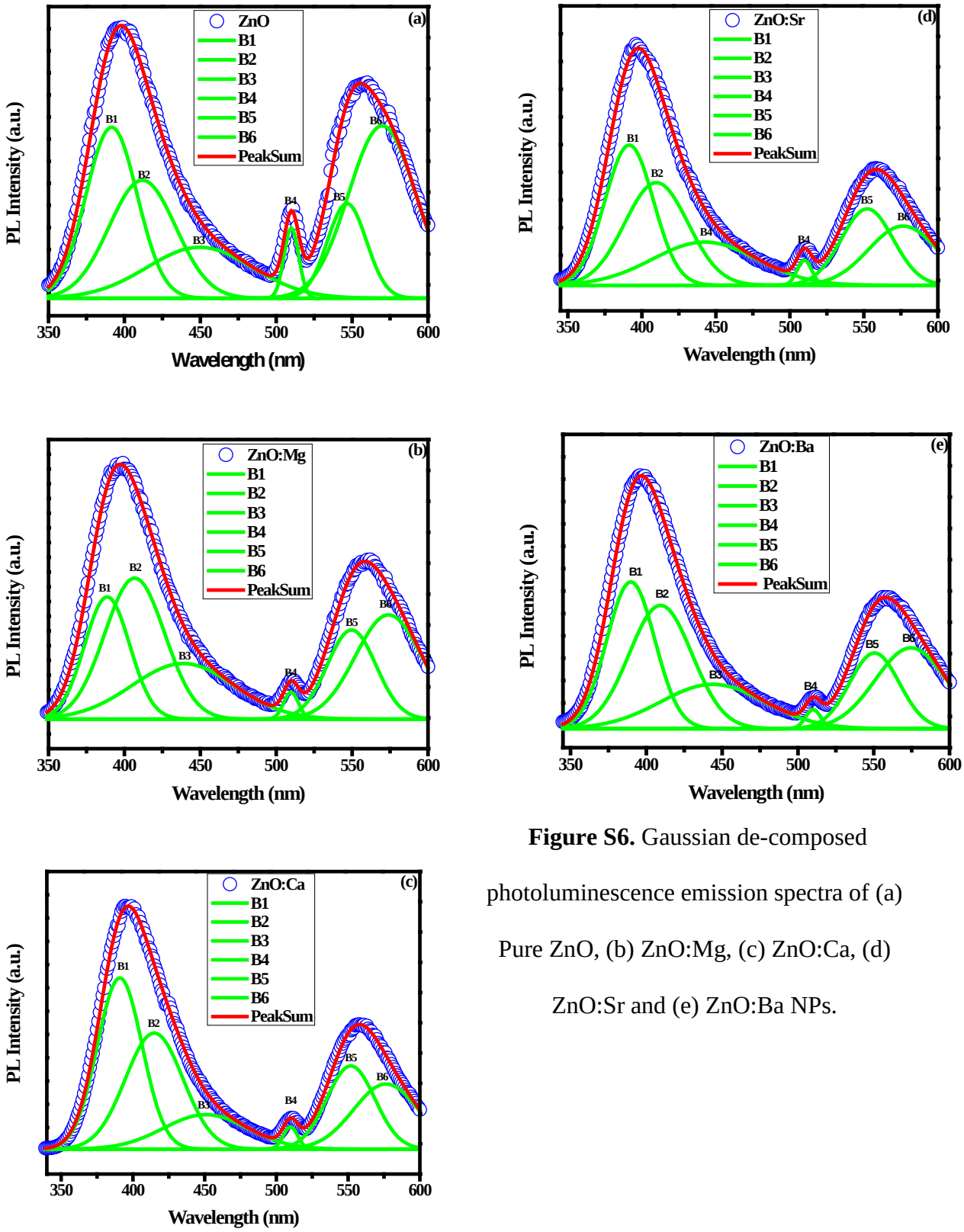

Figure S6. Gaussian de-composed photoluminescence emission spectra of (a) Pure ZnO, (b) ZnO:Mg, (c) ZnO:Ca, (d) ZnO:Sr and (e) ZnO:Ba NPs.