

SUPPLEMENTARY MATERIAL

Table 1S. Theoretical results obtained from the wurtzite-ZnO structure, lattice parameters (in Å), tetragonality factor (c/a) and band-gap (E_g in eV)

Wurtzite ZnO Structure			
a=b	c	c/a	E_g
3.290 ^a	5.233 ^a	1.591 ^a	3.11 ^a
3.249 ^b	5.204 ^b	1.601 ^b	-
3.166 ^c	5.070 ^c	1.601 ^c	-
3.266 ^d	5.247 ^d	1.606 ^d	3.76 ^d
3.290 ^e	5.227 ^e	1.589 ^e	12.66 ^e

^aThis work.

^bMössbauer measurement.¹

^cTheoretical (DFT/LDA+U).²

^dTheoretical (DFT/B3LYP).³

^eTheoretical (HF).³

Table 2S. Theoretical results calculated for indirect and direct band gaps (E_g in eV), wavelength (in nm), electromagnetic radiation range in relation to doping amount (in %)

Doping amount (%)	E_g	λ	Electromagnetic radiation
0.0	3.11 ($\Gamma - \Gamma$)	398.99	Ultraviolet A
6.12	2.91 (M – A)	426.20	UV-Visible (violet)
12.5	2.85 (L – Γ)	435.35	UV-Visible (violet)
25.0	2.83(L – Γ)	438.42	UV-Visible (violet)
37.5	2.97 (A – Γ)	417.78	UV-Visible (violet)
50.0	3.21 (A – Γ)	386.51	Ultraviolet A
62.5	3.99 ($\Gamma - \Gamma$)	310.95	Ultraviolet B
75.0	4.31 ($\Gamma - \Gamma$)	287.88	Ultraviolet B
87.5	4.90 ($\Gamma - \Gamma$)	253.35	Ultraviolet C
100	5.36 (SM – T)	231.46	Middle Ultraviolet

Figure 1S. Projected DOS for ZnO (a) and Ba-doped ZnO materials at 6.25% (b), 12.5% (c), 25% (d), 37.5% (e), 50% (f), 62.5% (g), 75% (h), 87.5% (i) e 100% (j)

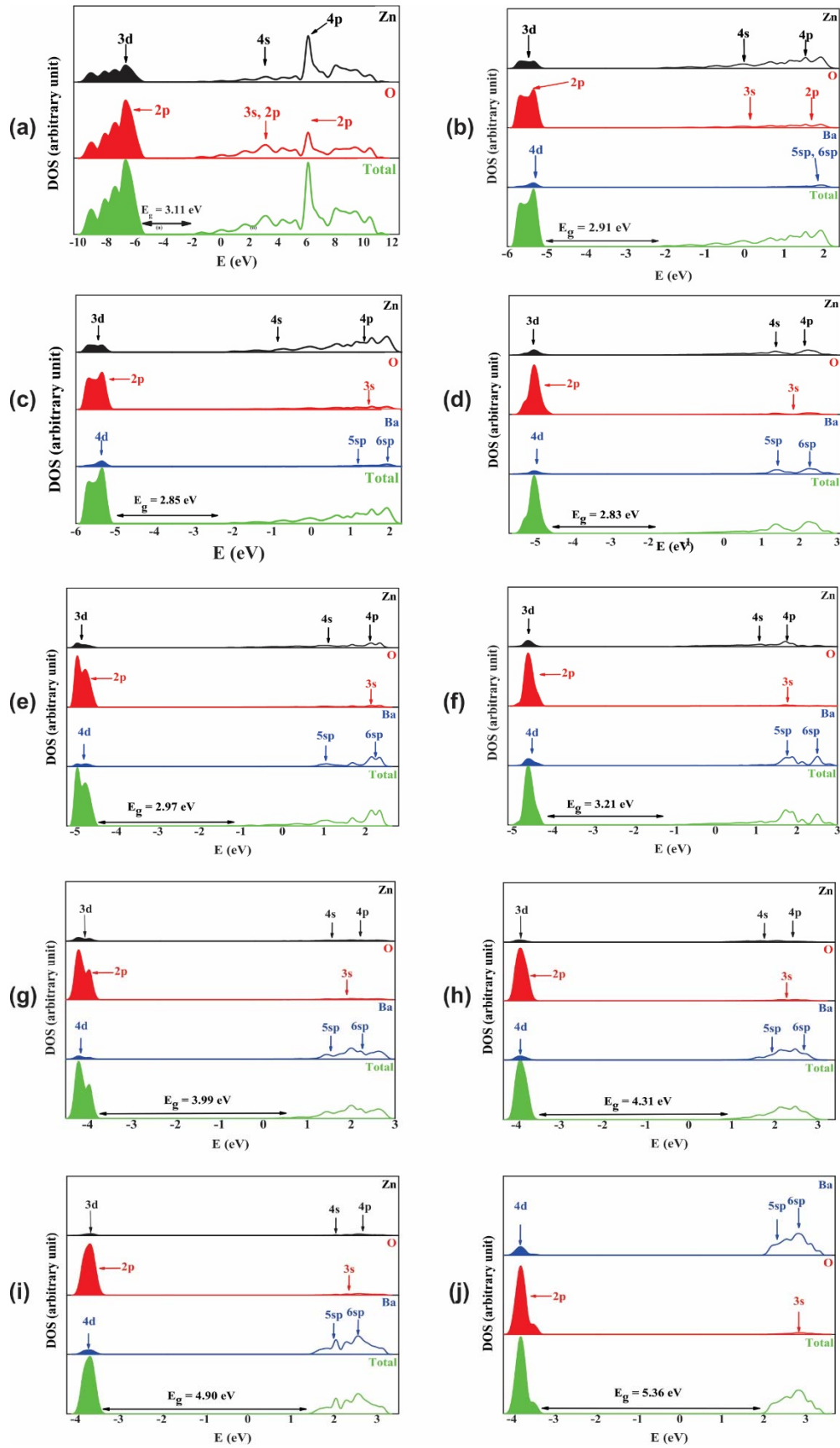
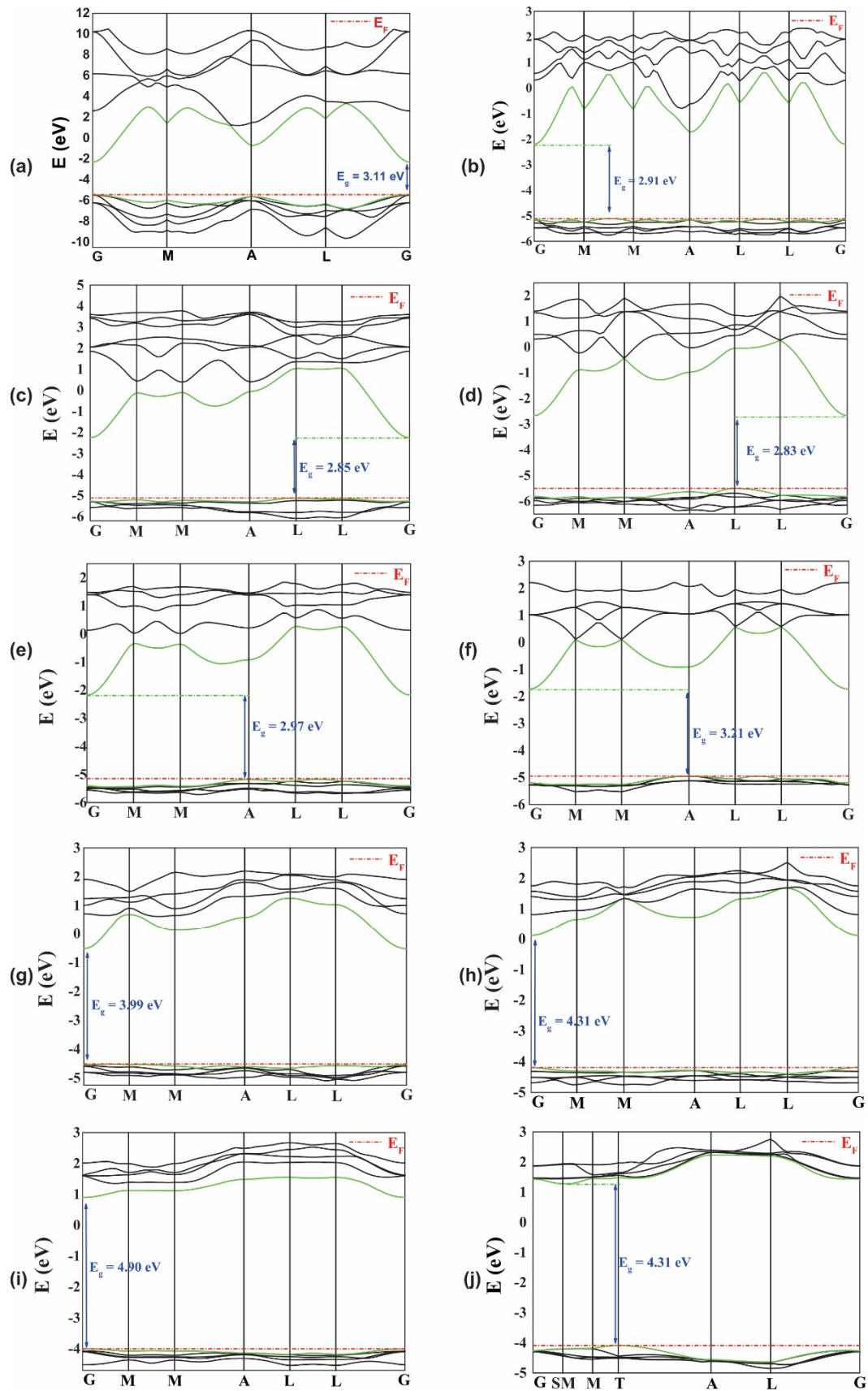


Figure 2S. Band Structure for ZnO (a) and Ba-doped ZnO materials at 6.25% (b), 12.5% (c), 25% (d), 37.5% (e), 50% (f), 62.5% (g), 75% (h), 87.5% (i) e 100% (j)



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