Electronic Supplementary Material (ESI) for RSC Advances.

Electronic structure and optical properties of $Zn(OH)_2$: LDA + *U* calculations and intense yellow luminescence

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Table S1 Optimized lattice constants and difference in volume (ΔV) for ZnO and $Zn(OH)_2$.

	a (Å)	*b* (Å)	*c* (Å)	ΔV (%)
ZnO	3.247	–	5.252	0.74
$Zn(OH)_2$	4.879	5.099	8.678	0.98

Table S2 Atomic populations (Mulliken) of ZnO and $Zn(OH)_2$.

	Species	s	p	d	Total	Charge (e)
ZnO	O	1.83	5.11	0.00	6.94	-0.94
	Zn	0.40	0.68	9.98	11.06	0.94
$Zn(OH)_2$	H	0.60	0.00	0.00	0.60	0.40
	O	1.82	5.17	0.00	6.99	-0.99
	Zn	0.30	0.53	9.99	10.82	1.18

Table S3 Bond populations and lengths of ZnO and $Zn(OH)_2$.

	Bond	Population	Length (Å)
ZnO	O–Zn ($// c$)	0.43	1.978
	O–Zn ($\perp c$)	0.39	1.986
$Zn(OH)_2$	H–O [a]	0.61	1.004
	H–O [b]	0.09	1.768
	O–Zn	0.38	1.982
	O–Zn	0.34	1.993
	O–Zn	0.36	2.002
	O–Zn	0.32	2.005

[a] within OH ion, [b] between OH ions

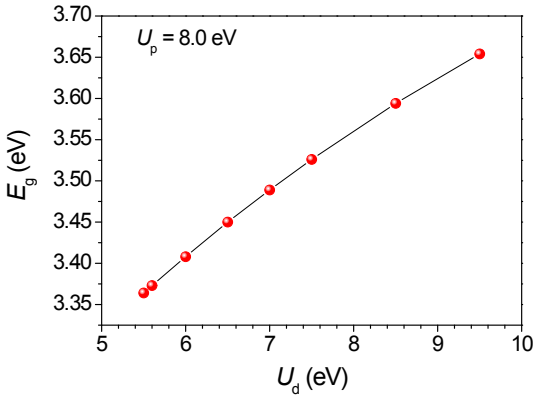

Figure S1 Variation of the E_g of ZnO as a function of U_d at a fixed U_p of 8.0 eV. Nearly linear increase of the E_g with U_d is observed in the LDA + U calculations.

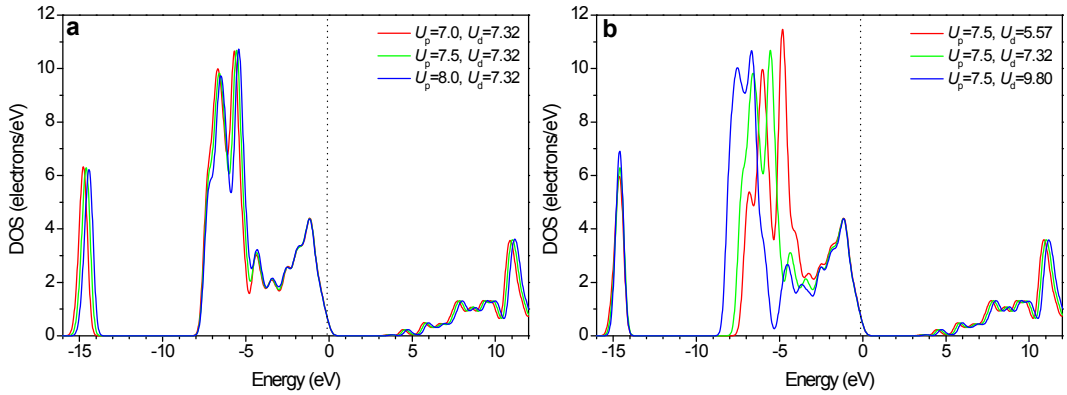

Figure S2. DOSs for ZnO calculated with LDA + U at fixed U_d (a) and U_p (b).

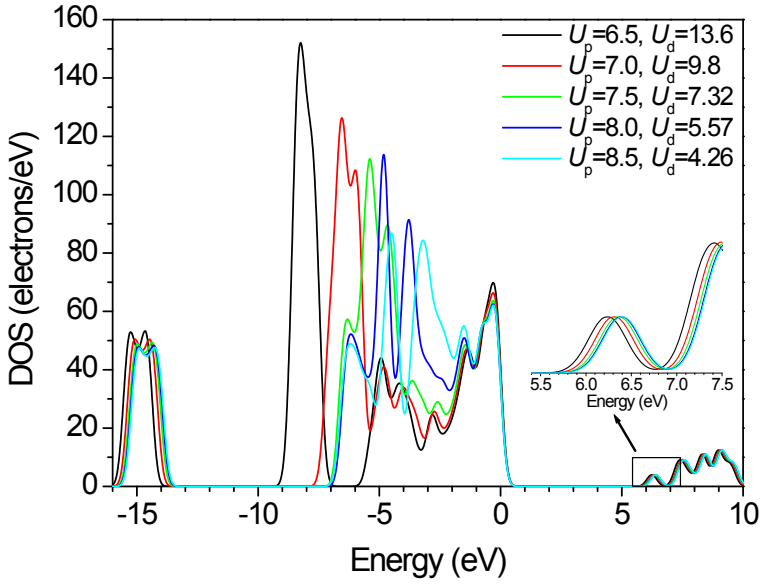

Figure S3. DOSs for $Zn(OH)_2$ calculated with LDA + U using various U parameters. The DOSs in the CB minimum is magnified as an inset.