

Supporting Information:

Optimization of the Electron Transport in Quantum Dot Light-Emitting Diodes by codoping ZnO with Gallium(Ga) and Magnesium(Mg)

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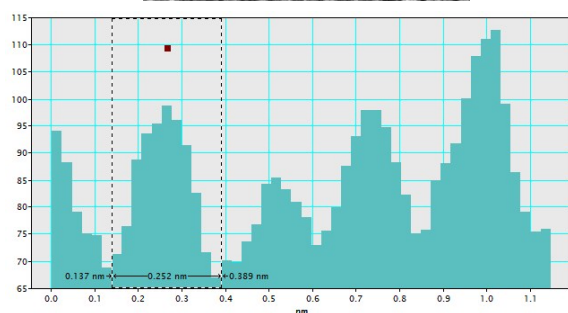
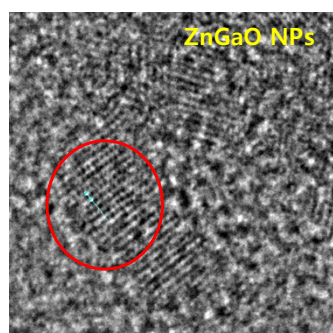
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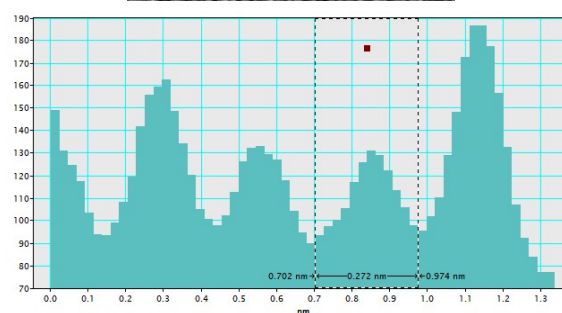
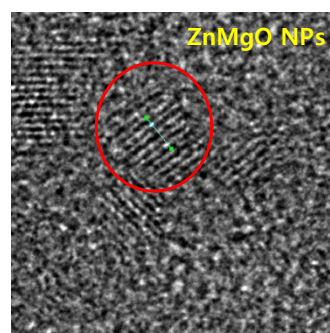
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(a)



(b)



(c)

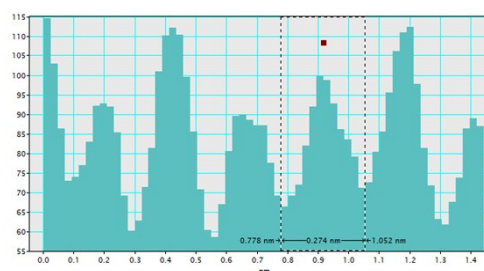
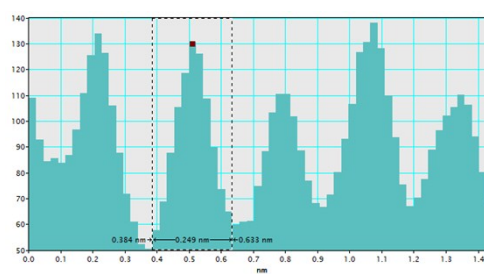
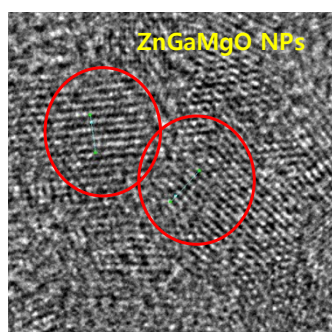


Figure S1. HRTEM images and a line profile on the (a) ZnGaO, (b) ZnMgO, and (c) ZnGaMgO NPs.

The donor concentration (N_D) of four materials is calculated using to BM shift equation: The Fermi levels of four materials (ZnO, ZnGaO, ZnMgO, and ZnGaMgO NPs) are located about the CBM with energy as high as 0.13-0.46 eV, which indicates that energy levels are degenerate. This degeneration is observed as the bandgap widens in the semiconductor, and the concentration can be determined by the well-known Burstein-Moss shift equation (1).

$$\Delta E_{BM} = E_F - E_{CBM} = \left(\frac{h^2}{8\pi^2 m_{eh}^*} \right) (3\pi^2 n)^{\frac{2}{3}}, \quad (1)$$

where m_{eh}^* , E_F , E_{CBM} , and n are the electron-hole reduced mass (0.19 m_e), Fermi level, minimum energy of the conduction band, and carrier concentration, respectively. The optical bandgap of 3.50, 3.58, 3.75, and 3.61 eV measured from UV-vis absorption (figure 4(a)), corresponding to $\Delta E_{BM} = 0.13, 0.26, 0.46$, and 0.38 eV. Using ΔE_{BM} , the donor concentration (N_D)

Donor concentration (N_D)	
ZnO	$1.76 \times 10^{19} \text{ cm}^{-3}$
Zn _{0.88} Ga _{0.12} O	$4.99 \times 10^{19} \text{ cm}^{-3}$
Zn _{0.86} Mg _{0.14} O	$1.17 \times 10^{20} \text{ cm}^{-3}$
Zn _{0.87} Ga _{0.1} Mg _{0.03} O	$8.83 \times 10^{19} \text{ cm}^{-3}$

of four materials can be deduced according to equation (1). Calculated values are as below.

Table 1. Atomic Concentration (%) of ZnO, ZnGaO, ZnMgO, and ZnGaMgO NPs as measured by XPS and the relative concentration of Ga and Mg elements vs Zn element.

	C1s	O1s	Mg1s	Zn2p ³	Ga2p ³	Total
ZnO	19.7	39.7	-	40.6	-	100
ZnGaO	20.3	41.2	-	33.9	4.6	100
ZnMgO	25.6	41.9	4.7	27.8	-	100
ZnGaMgO	22.1	41.5	0.9	31.7	3.8	100

	Mg	Zn	Ga	Total
ZnGaO	-	88	12	100
ZnMgO	14	86	-	100
ZnGaMgO	3	87	10	100

Table 2. Energy offsets formed at the interface of QDs/ETLs and ETLs/Al electrode.

	ΔG (eV)		
	CBM_{ETL}/Al (Schottky barrier)	CBM_{ETL}/CBM_{QD}	VBM_{ETL}/VBM_{QD}
ZnO	1.09	0.99	0.21
$Zn_{0.88}Ga_{0.12}O$	0.44	0.34	0.94
$Zn_{0.87}Ga_{0.1}Mg_{0.03}O$	0.41	0.31	1.00
$Zn_{0.86}Mg_{0.14}O$	0.25	0.15	1.30