Supplementary Information

Reactivity-Matched Synthesis of Monodisperse $Ag(In,Ga)S_2$ QDs with Efficient Luminescence

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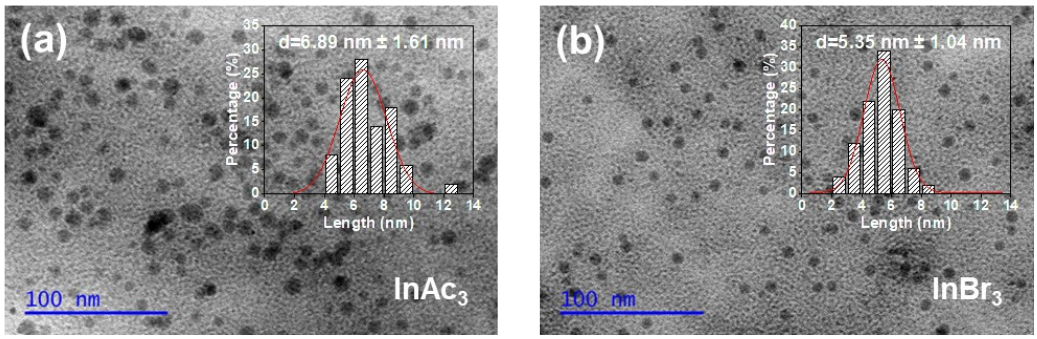

Fig. S1 TEM images and the corresponding size distribution histograms of the AIGS QDs synthesized using $InAc_3$ and $InBr_3$, respectively.

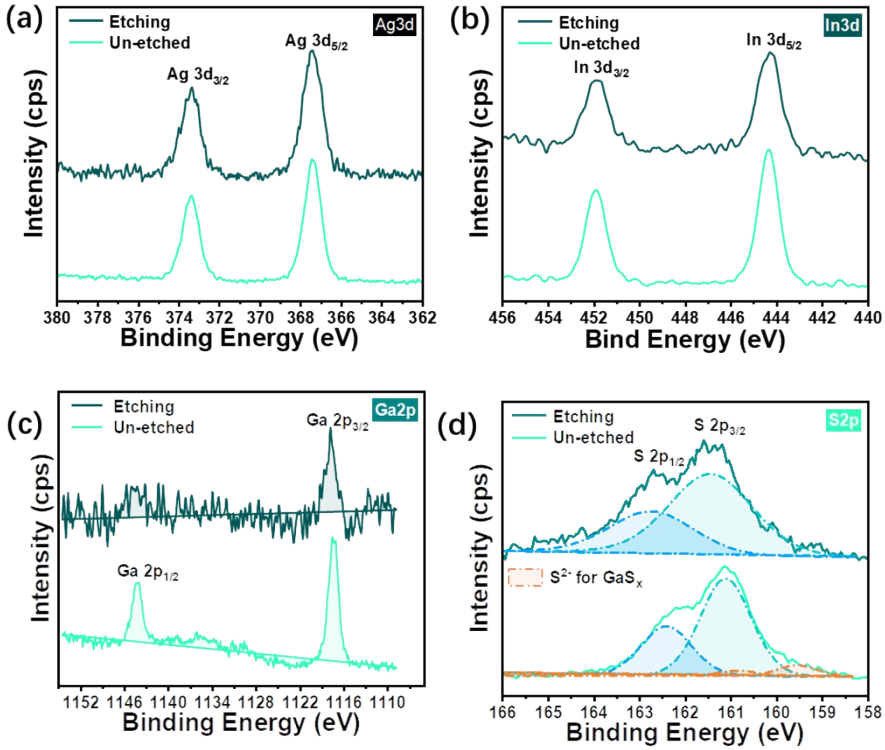

Fig. S2 XPS spectra of AIGS@GaS_x core/shell QDs for (a) Ag 3d, (b) In 3d, (c) Ga 2p, and (d) S 2p regions synthesized using InI_3 before and after etching.

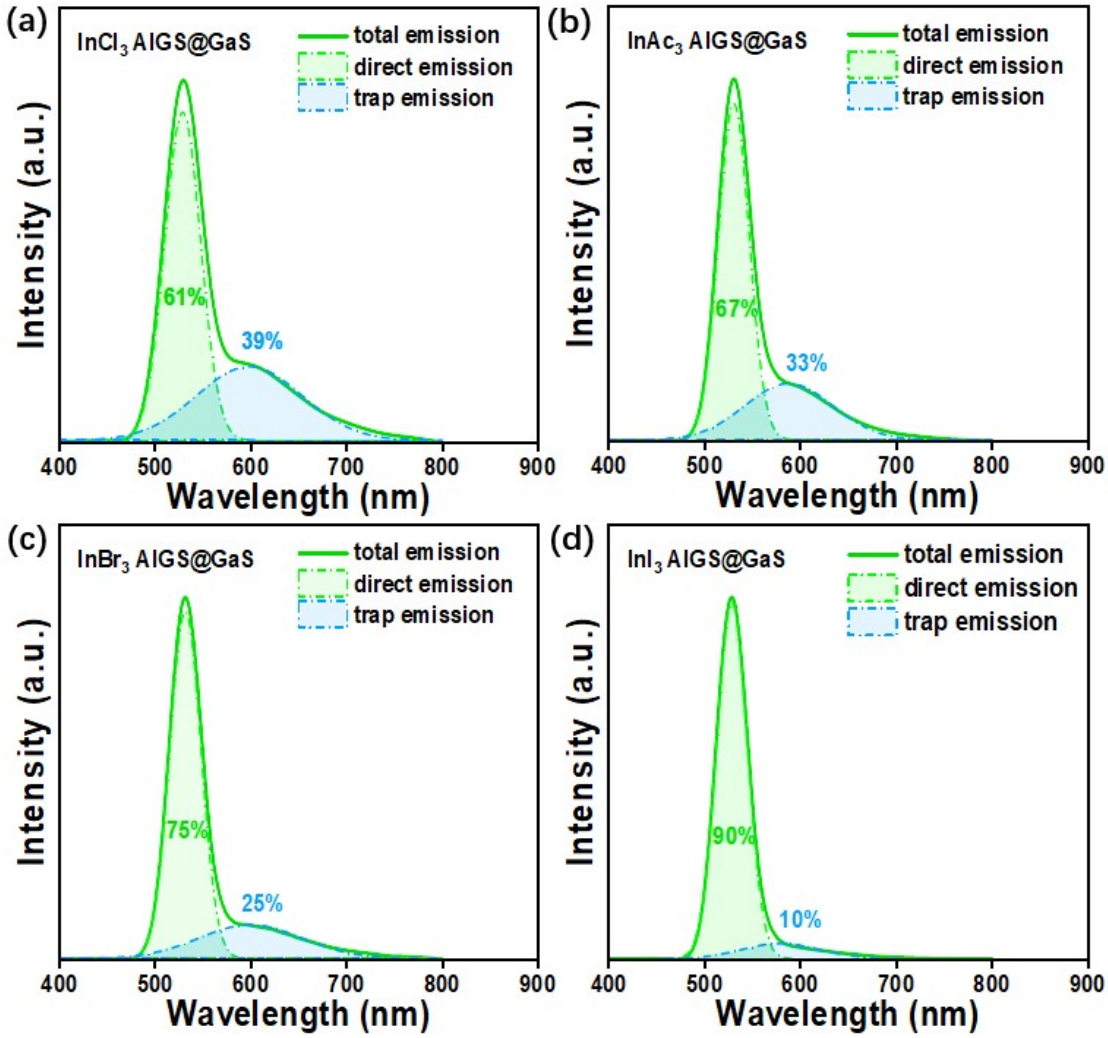

Fig. S3 Fitted PL spectra of the AIGS QDs synthesized using (a) $InCl_3$, (b) $InAc_3$, (c) $InBr_3$, and InI_3, respectively.

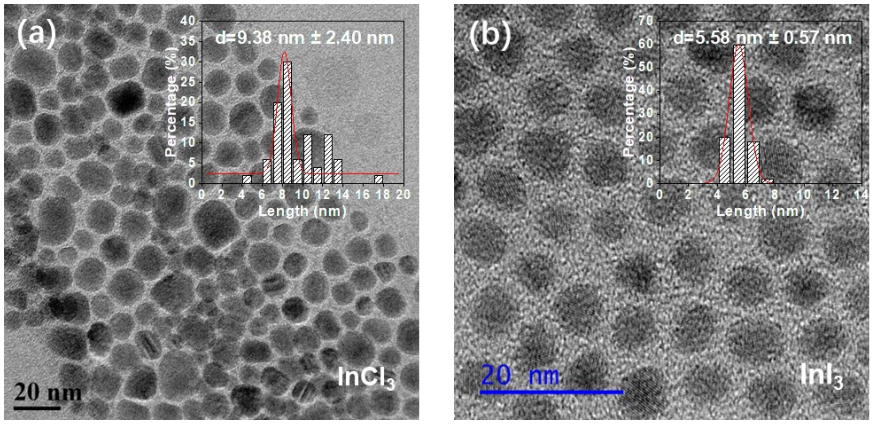

Fig. S4 TEM images of the AIGS@GaS_x QDs synthesized using $InCl_3$ and InI_3, respectively.

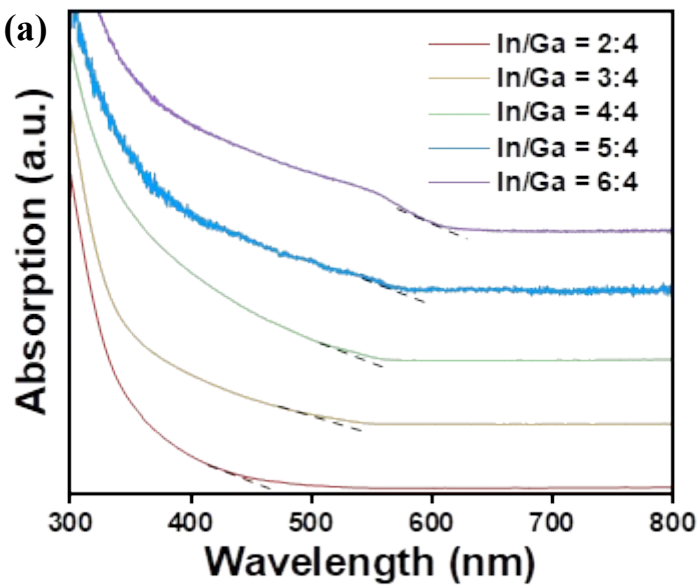

Fig. S5 Absorption curves of AIGS@GaS_x core/shell QDs with different In/Ga ratios.

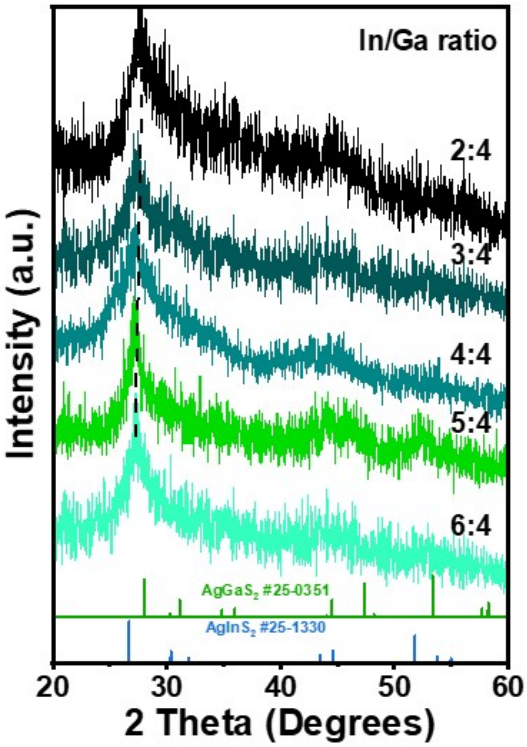

Fig. S6 XRD spectra of the AIGS/GaS_x core/shell QDs with In/Ga molar ratios of 2:4, 3:4, 4:4, 5:4, and 6:4 synthesized with the same metal salt InI_3.

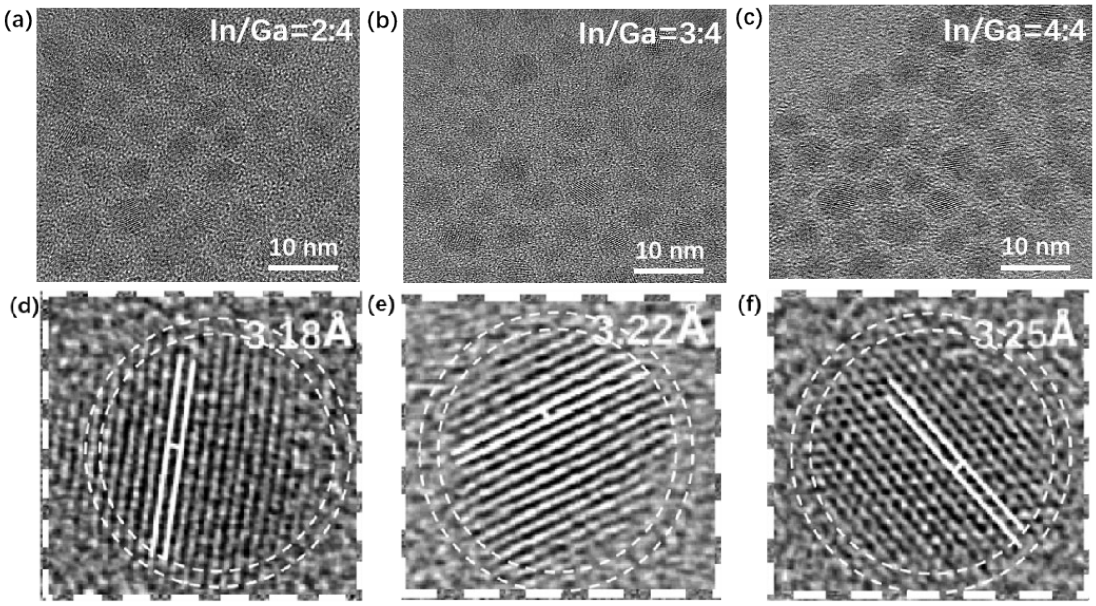

Fig. S7 TEM image of the AIGS/GaS_x core/shell QDs with In/Ga molar ratios of (a) 2:4, (b) 3:4, (c) 4:4, HRTEM image of the AIGS/GaS_x core/shell QDs with In/Ga molar ratios of (d) 2:4, (e) 3:4, and (f) 4:4.

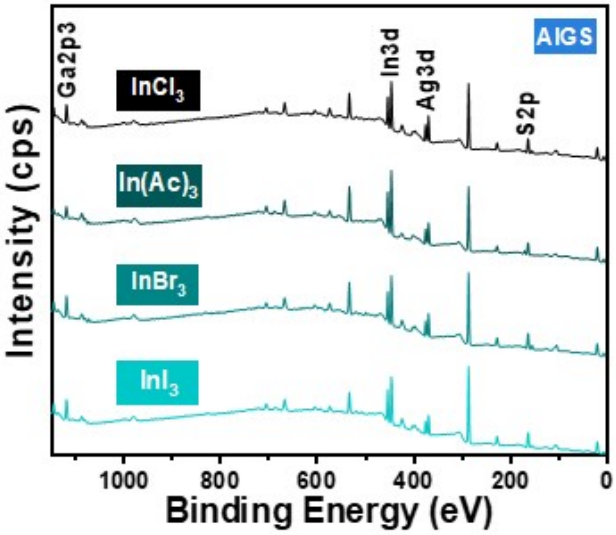

Fig. S8 XPS spectra of AIGS QDs synthesized using $InCl_3$, $InAc_3$, $InBr_3$, and InI_3, respectively.

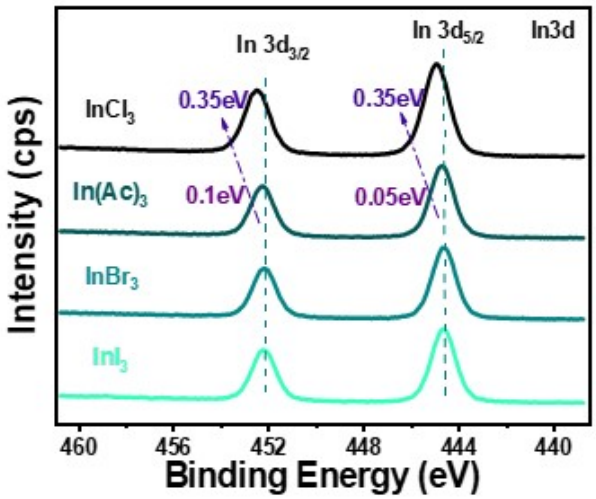

Fig. S9 XPS spectra of AIGS QDs for In 3d regions synthesized using difference In sources.

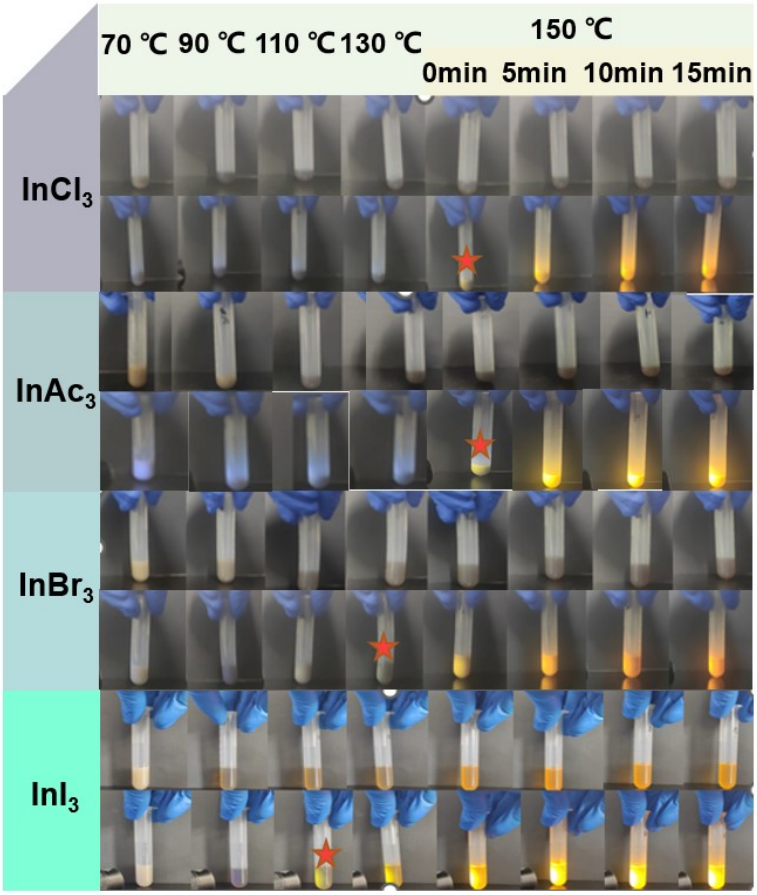

Fig. S10 Photographs for reaction stage under white light (upper photos) and UV light (bottom photos) extracts from 70 ℃ to 150 ℃ 15 min of AIGS QDs synthesized using $InCl_3$, $InAc_3$, $InBr_3$, and InI_3, respectively.

Table S1. Elements Hard and Soft Acid and Base (HSAB) diagram.

Acid \ Base		Hard base	Junction base	Soft base
		CH_3COO^-、Cl^-	Br^-	I^-
Hard acid	In^{3+}	Strong bond	Relatively strong bond	Weak bond

Table S2. Calculated bond formation energies from $In(A)_3$ to In^{3+} (A = Cl^-, Ac^-,

Br^-, I^-)

	$InCl_3$	$InAc_3$	$InBr_3$	InI_3
E_{form}	1.01 eV	2.59 eV	0.86 eV	0.50 eV

Table S3. Average lifetimes and radiative composite and nonradiative occupancies of AIGS QDs synthesized using $InCl_3$, $InAc_3$, $InBr_3$, and InI_3, respectively.

AIGS	$<\tau_{av}>$ (ns)	τ_1 (ns)	τ_2 (ns)	f_1	f_2
$InCl_3$	177.92	28.04	214.55	73.19%	26.81%
$InAc_3$	175.41	34.79	203.90	57.69%	42.31%
$InBr_3$	181.94	38.52	208.46	45.21%	54.79%
InI_3	197.24	42.70	223.08	38.22%	61.78%

Table S4. Element atom % of QD and etch-QD analyzed by XPS.

Sample	**Element atom %**				
	Ag	**In**	**Ga**	**Ag+In+Ga**	**S**
QD	11.88	5.49	17.43	34.80	65.20
Etch-QD	18.18	9.09	5.84	33.11	66.89

Table S5. Average lifetimes and radiative composite and nonradiative occupancies

of AIGS@GaS_x QDs synthesized using $InCl_3$, $InAc_3$, $InBr_3$, and InI_3, respectively.

AIGS@GaS_x	$<\tau_{av}>$ (ns)	τ_1 (ns)	τ_2 (ns)	τ_3 (ns)	f_1	f_2	f_3
$InCl_3$	106.03	6.89	41.83	207.60	5.01%	33.37%	61.62%
$InAc_3$	99.01	7.85	44.54	189.75	8.09%	37.66%	54.25%
$InBr_3$	84.63	5.92	35.51	133.64	7.45%	46.38%	46.17%
InI_3	76.66	4.35	26.86	157.10	8.55%	54.69%	36.76%

Table S6. Summary of properties based on I-III-VI and derivative QDs.

QDs	PL (nm)	FWHM (nm)	Colour	PLQY (%)	Ref
AIS@GaS_x	600	30	Yellow	56%	1
AIS@GaS_x	~580	~33	Yellow	72.3	2
AIS@GaS_x	560	45	Yellow	26.7	3
AIS@GaS_x	530	~37	Green	40	4
AIS@GaS@ZnS	575	~48	Yellow	~60	5
AIGS@GaS_x	530	41	Pure-Green	~28	6
AIGS@GaS_x	568	36	Yellow	71	7
AIGS@GaS_x	518	36	Green	68	8
AIGS@GaS_x	543	37	Green	99	9
AIGS@GaS_x	528	31	Pure-Green	53	9
AIGS@AGS	517	30	Green	96	10
AIGS@GaS_x	**530**	**31**	**Pure-Green**	**90**	**This work**

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