

## Supplementary Materials:

### Bright, Efficient, and Color-stable Violet ZnSe-Based Quantum Dots Light-Emitting Diodes

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### Experimental details of synthesis of ZnSe quantum dots

#### Chemicals

All reagents were used as received without further experimental purification. Zinc oxide (ZnO, 99.99% powder), sulfur (S, 99.98%, powder), 1-octadecene (ODE, 90%), oleic acid (OA, 90%), octanethiol (OT, 98%) and selenium (Se, 99.99%, powder) were purchased from Aldrich. hexanes (analytical grade), paraffin oil (analytical grade), and methanol (analytical grade) were obtained from Beijing Chemical Reagent Ltd., China.

#### Preparation of precursors

#### Stock solution for Zn precursor

A mixture (20 mL in total) of ZnO (0.16274 g, 2 mmol), oleic acid (8 mmol, 2.256 g), and 17.5 mL paraffin oil was loaded in a 50 mL three-neck flask and heated to 300 °C under nitrogen to obtain a colorless clear solution.

#### **Solution for Se precursor**

It was made by degassing Se (0.1578 g, 2 mmol), 20 mL of ODE in a 50 mL three-neck flask, then it was heated to 220 °C for 180 min under nitrogen. During this procedure, the color of the precursor changed from transparent to orange, red, and finally turned into yellow.

#### **Synthesis of ZnSe quantum dots**

2 mL (0.2 mmol) Se precursor and 8 g paraffin oil was heated to 300 °C under nitrogen gas flow in a 100 mL flask. Next, 1.3 mL (0.2 mmol) Zn Precursor solution was injected and temperature was lower to 280°C for QD growth. Aliquots were taken at different time intervals, and UV-vis and PL spectra were recorded for each aliquot (Figure S1). PL spectra covered from 400 nm to 450 nm (Figure S1).

#### **Synthesis of ZnSe/ZnS core-shell QDs with different temperature**

2 mL (0.2 mmol) Se precursor and 8 g paraffin oil was heated to 300 °C under nitrogen gas flow in a 100 mL flask. Next, 1.3 mL (0.2 mmol) Zn Precursor solution was injected and temperature was lowered to 280 °C for ZnSe QDs growth. When the reaction maintained for 5 min (Figure S1), the reaction temperature was set at 240 °C, or 260 °C, or 280 °C, or 300 °C, or 340 °C, without any purification steps, then 2 mL OT mixed with 20 mL of Zn precursor was added at a rate of 6 mL/h. All the shell growth processes lasted for 4 h. Aliquots of QDs were taken during the reaction to

analyze the development of ZnSe/ZnS core/shell QDs. After the reaction was completed, the temperature was cooled down to room temperature and the QDs were purified using acetone or methanol.

### **Stability test of ZnSe/ZnS core/shell quantum dots**

To check the stability of ZnSe/ZnS core/shell quantum dots through purification, the quantum dots were precipitated from growth solution and dispersed in hexane as described above. Then they were subsequently subjected to multiple “purification” steps in which they were completely precipitated with methanol followed by re-dispersion in hexane. This process was repeated up to sixteen times. PL QYs were measured in growth solution, as well as after each precipitation/re-dispersion cycle (Figure 4B).

### **Detailed calculations of power efficiency and external quantum efficiency:**

There are two parameters to determine the efficiency of QD-LEDs: current efficiency ( $\eta_A$ ) and power efficiency ( $\eta_P$ ). Current efficiency ([cd/A]) or luminance efficiency which is defined as the ratio of luminance ( $L$ ) to the injection current density to QD-LEDs,  $J_D$ , can be expressed as:

$$\eta_A = \frac{L}{J_D}$$

Power efficiency ([lm/W]) is defined as the ratio of the output luminous flux to the input power of QD-LEDs. Similar to current efficiency,  $\eta_P$  can be expressed as:

$$\eta_P = \frac{L \cdot A \cdot \pi}{J_D \cdot A \cdot V} = \frac{L}{J_D} \cdot \frac{\pi}{V}$$

where  $V$  ([V]) is the applied voltage to QD-LEDs.

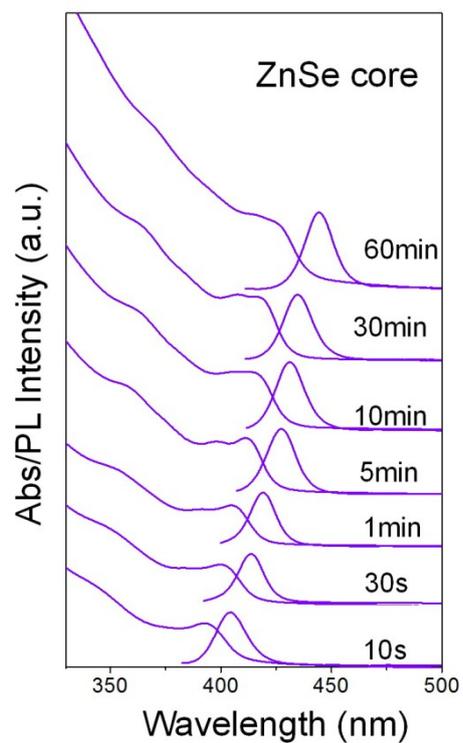
External quantum efficiency ( $\eta_{EQE}$ ) mentioned in the previous section, which is the ratio of the number of photons emitted from the QD-LEDs to the number of charge carriers injected into the device, can be expressed as:

$$\eta_{EQE} = \frac{\int \frac{I(\lambda)}{hc/\lambda} d\lambda}{J_D A / q} = \frac{q}{hc} \cdot \frac{\int \lambda I(\lambda) d\lambda}{J_D A}$$

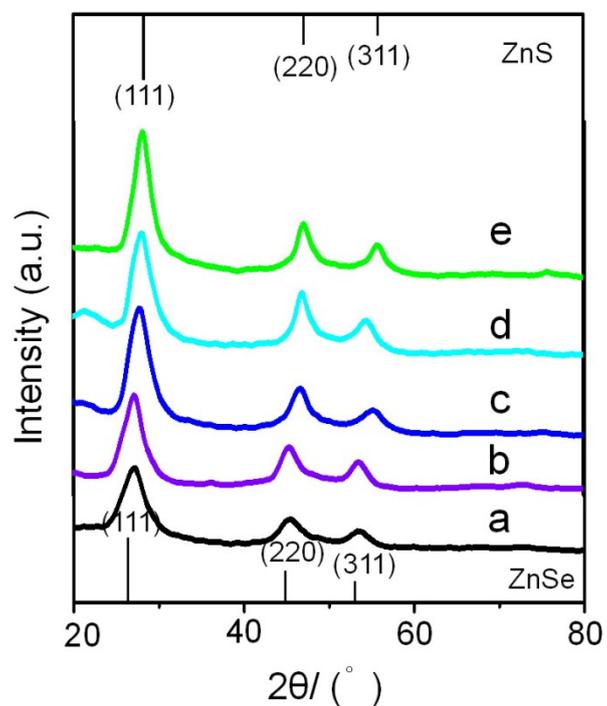
where  $q$  is the electric charge,  $h$  is Planck's constant, and  $c$  is speed of light. By

Combining with the above equations, it can be derived as:

$$\eta_{EQE} = \frac{q}{hc} \cdot \frac{\int \lambda I(\lambda) d\lambda}{J_D A} = \frac{q}{hcf} \cdot \frac{\int \lambda S(\lambda) d\lambda}{\xi} \cdot \frac{I_{det}}{J_D A}$$



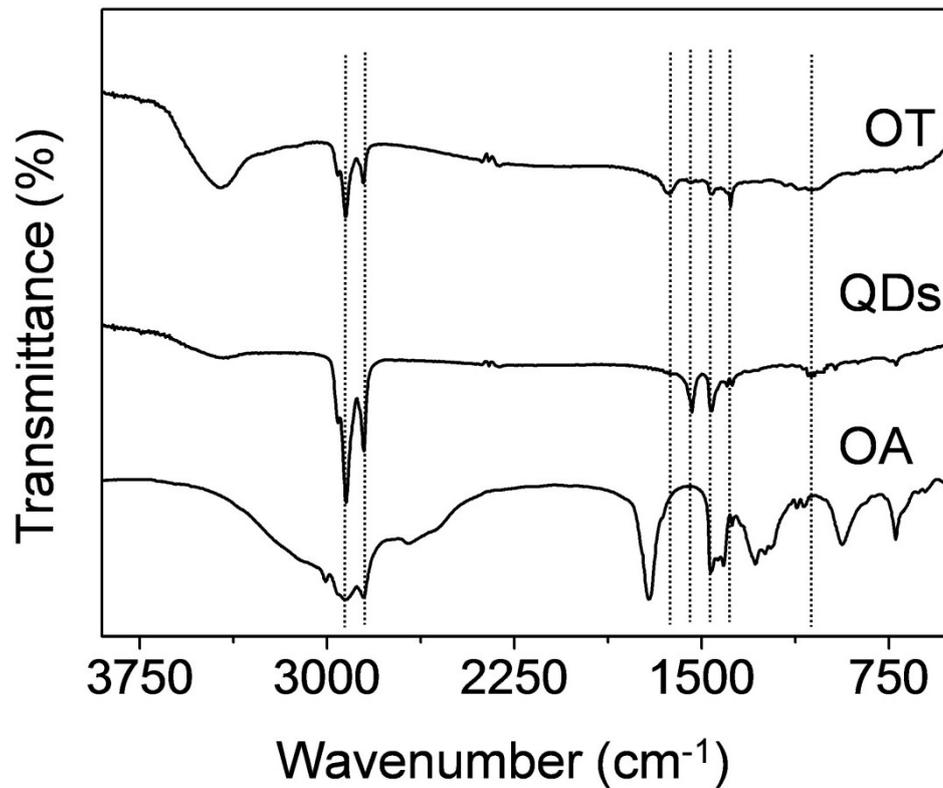
**Figure S1.** Time evolution of the absorption and PL spectra of ZnSe QDs synthesized at 300 °C. The numbers mentioned on the right of each spectrum indicate the reaction time.



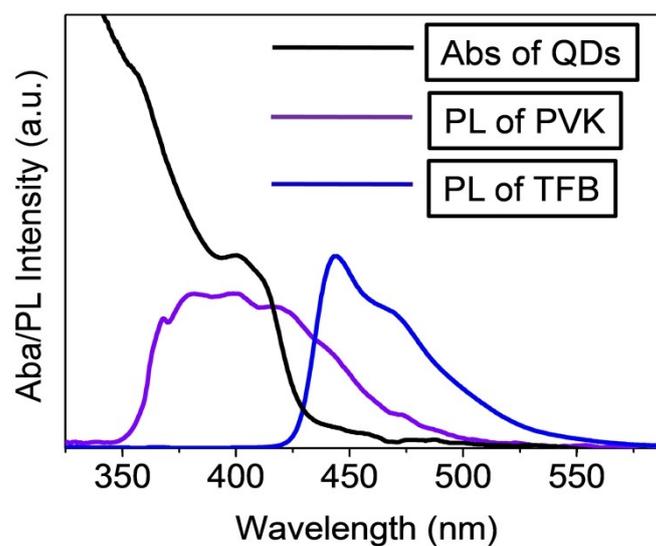
**Figure S2.** Powder XRD patterns of ZnSe cores and ZnSe/ZnS core/shell QDs with different growth time. XRD patterns of ZnSe cores for (a) 3 min and (b) 10 min, respectively; and XRD patterns of ZnSe/ZnS with shell growth time of 1 (c):h; (d): 2 h; and (e): 4 h. For comparison, the standard powder diffractions of cubic ZnSe and ZnS bulk crystals are provided.

**Table S1.** The detailed information of QYs, PL peaks, and FWHMs with different shell growth times and temperatures.  $T_G$ : ZnS shell growth temperature; PL  $\lambda$  0, 1, 2, 3: PL peak of ZnSe core, ZnSe/ZnS-1h, ZnSe/ZnS-2h, ZnSe/ZnS-4h; FWHM 0, 1, 2, 3: FWHM of ZnSe, ZnSe/ZnS-1h, ZnSe/ZnS-2h, ZnSe/ZnS-4h; QY 0, 1, 2, 3: QY of ZnSe, ZnSe/ZnS-1h, ZnSe/ZnS-2h, ZnSe/ZnS-4h.

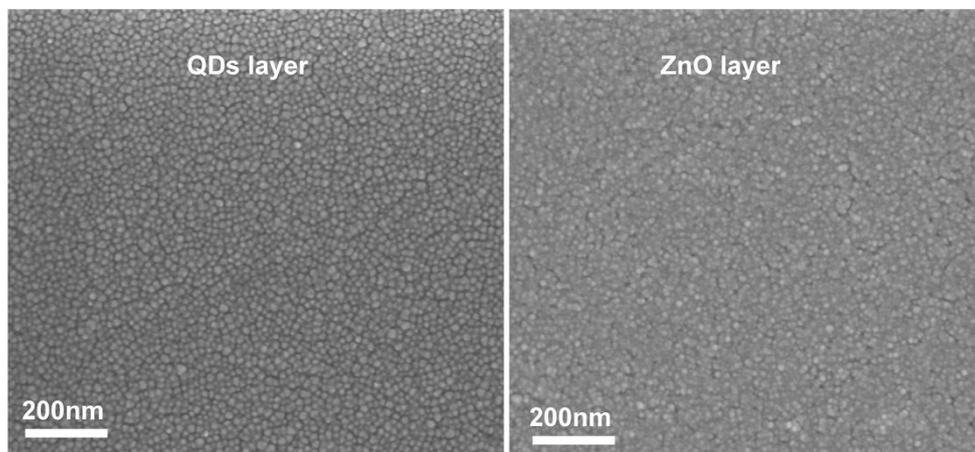
Core information			Shell growth temperature $T_G$ (°C)	Information of growth shell for 1h (ZnSe/ZnS-1h)			Information of growth shell for 2h (ZnSe/ZnS-2h)			Information of growth shell for 4h (ZnSe/ZnS-4h)		
PL $\lambda$ 0 (nm)	FWHM 0 (nm)	QY 0 (%)		PL $\lambda$ 1 (nm)	FWHM 1 (nm)	QY 1 (%)	PL $\lambda$ 2 (nm)	FWHM 2 (nm)	QY 2 (%)	PL $\lambda$ 3 (nm)	FWHM 3 (nm)	QY 3 (%)
423	18	41	240	425	18.3	48	427	21	37	429	25.2	24
423	18	41	260	426	18.2	61	429	21.5	47	430	24.3	32
423	18	41	280	426	18.2	60	427	18.7	51	430	18.5	51
423	18	41	300	426	17	58	426	17.6	73	425	17.2	69
423	18	41	320	425	16.8	66	426	16.3	79	424	16.6	83
423	18	41	340	422	18.8	67	420	21.4	69	418	27.8	71



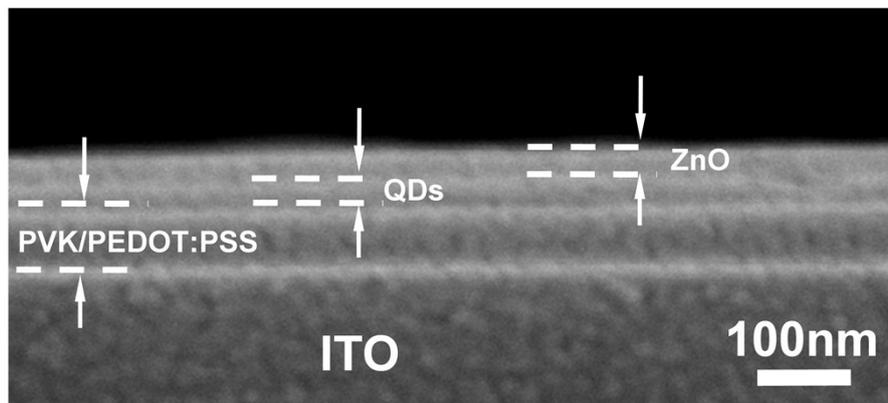
**Figure S3.** FTIR spectra of oleic acid (OA), QDs, and octanethiol (OT) which indicate the major surface ligands of QDs were OT molecules.



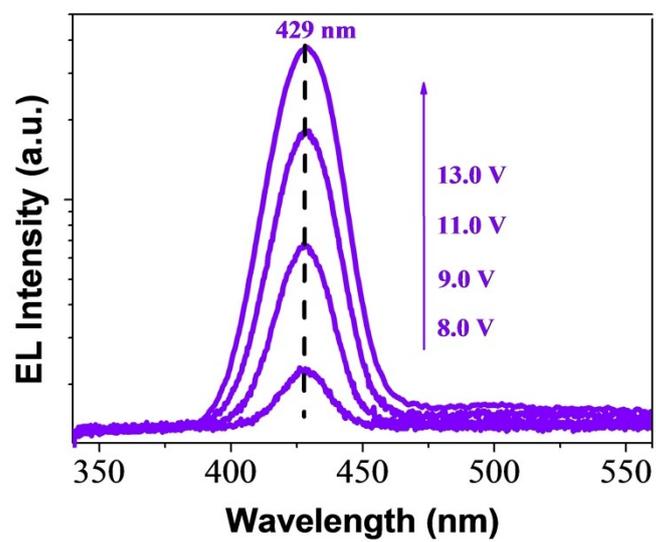
**Figure S4.** Absorption spectra of ZnSe/ZnS QDs in hexanes, and PL spectra of PVK and TFB in chlorobenzene are presented in solid lines with color of black, purple and blue, respectively.



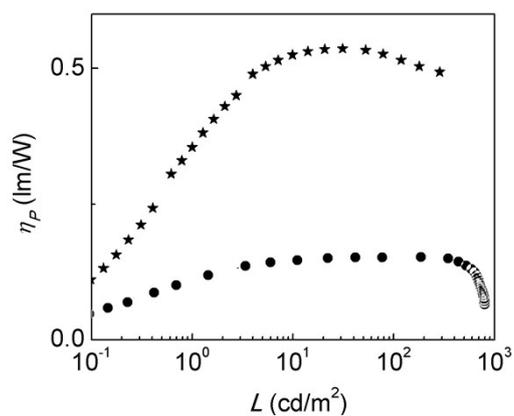
**Figure S5.** Surface SEM images of uniformly, compactly packed emitting layer of ZnSe/ZnS QDs and electron transport layer of ZnO NPs.



**Figure S6.** Cross-sectional SEM images of ITO/PEDOT:PSS/PVK/QDs/ZnO.



**Figure S7.** The corresponding EL spectra of Figure 5D at half-exponential coordinates.



**Figure S8.** Power efficiency–Luminance characteristics of violet QD-LEDs having the ZnSe/ZnS core-shell QDs synthesized with different S sources of S-ODE (●) and octanethiol (★).