Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

Continuous synthesis of high quality CdSe quantum dots in supercritical fluids

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Figure S1: Absorbance and PL spectra of CdSe QDs

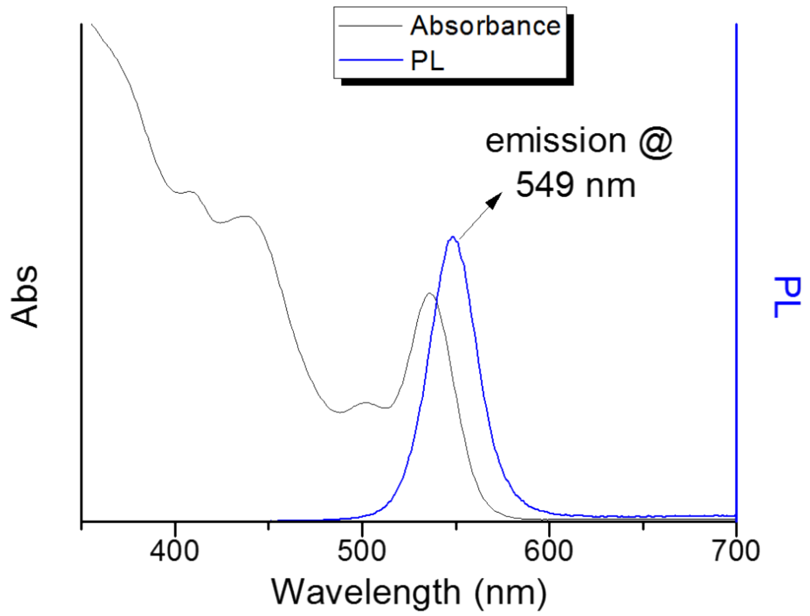
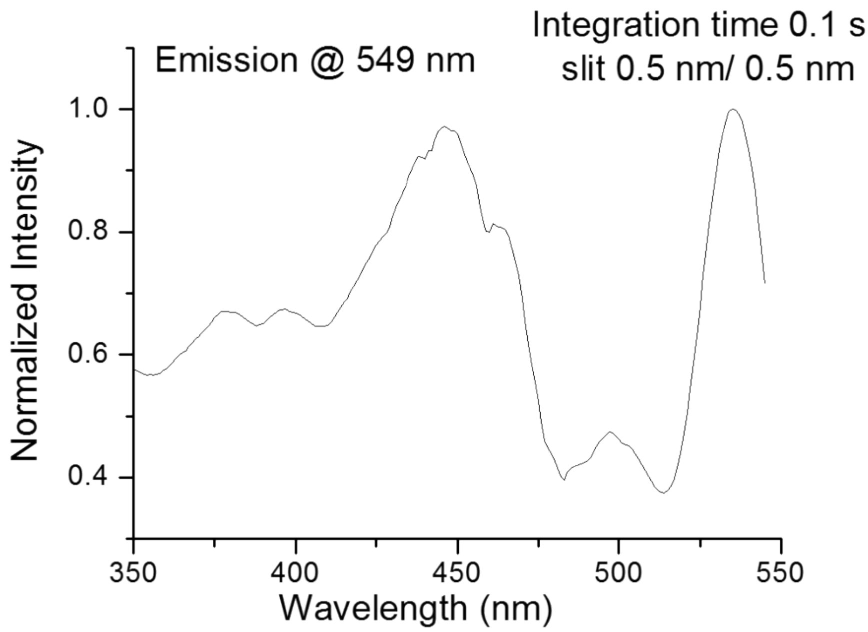
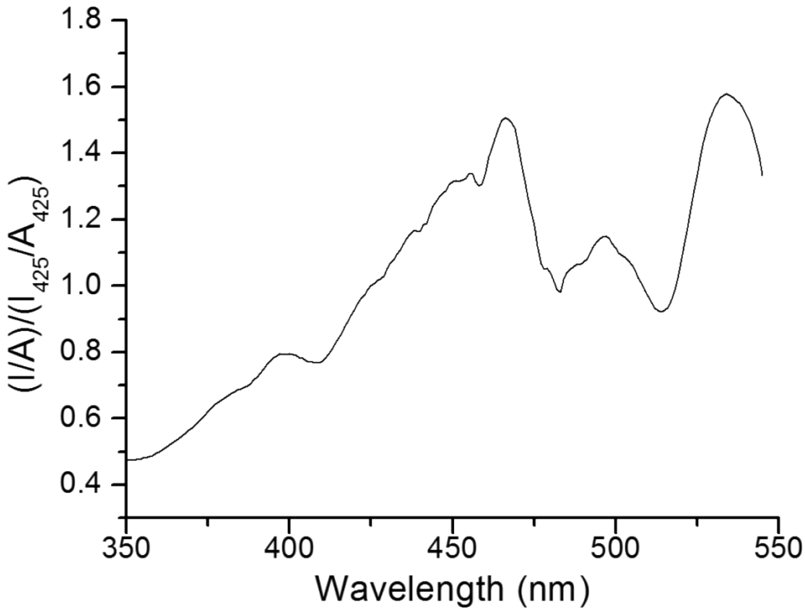


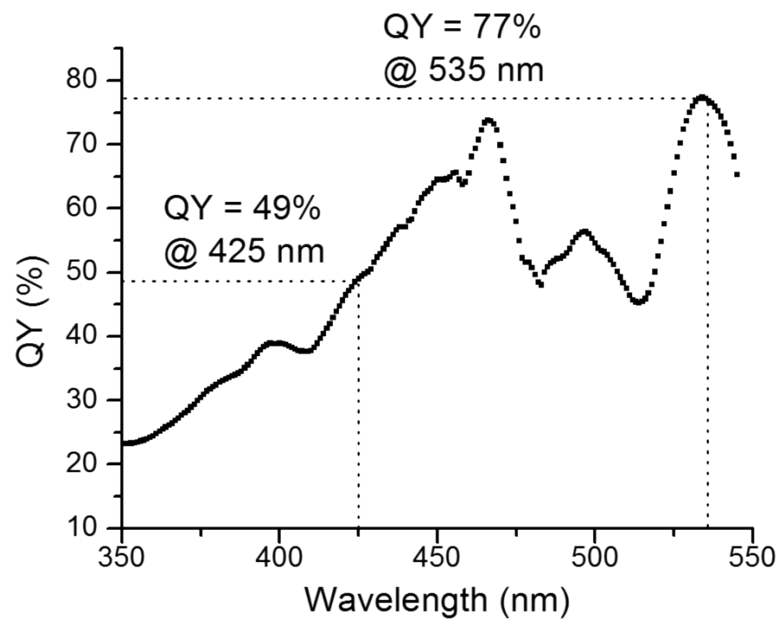
Figure S2: Excitation spectra of CdSe QDs



<u>Figure S3: Ratio of Intensity in the excitation spectra and absorbance vs wavelength of CdSe QDs</u>



<u>Figure S4: Quantum Yield vs wavelength of excitation of CdSe QDs</u>



Example of calculation of the CdSe QDs concentration obtained in supercritical fluids (case of CdSe QD558 – T = 250°C, R_t = 60s)

(Method demonstrated in: W. W. Yu, L. Qu, W. Guo and X. Peng, *Chem. Mater.,* 2003, **15**, 2854.)

The calculation is based on the Lambert-Beer's Law, $A = \varepsilon CL$.

First, the 0.2 mL of the QDs initial solution is diluted to 3 mL for absorption measurements.

Then, the sizes of the quantum dots can be estimated from the absorption and PL peaks (here D = 2.9 nm). Therefore, ε can be estimated as:

$\varepsilon = 5857 (D)^{2.65}$ (D = diameter of CdSe NCs)

$= 5857 (2.9)^{2.65}$

$= 98407\ M^{-1}cm^{-1}$

Finally, given that the absorbance value at first excitonic peak (544 nm) is equal to 0.48 and that L = 1 cm, we can calculated C:

$C_{CdSemol} = 4.87 \times 10^{-6}$ M

The total weight of a CdSe QDs can be estimated as:

$C_{CdSewt} = [(4/3) \times \pi \times r^3] \times \rho_{CdSe} \times C_{CdSemol} \times 6{,}023 \times 10^{23}$ g/L

since $\rho_{CdSe} = 5810\ kg.m^{-3}$ and r = 2,9 / 2 = 1,45 nm

Therefore, the concentration in mg/mL is: 0,218 mg/mL

Taking into the initial dilution factor:

C_{CdSe} = 3,264 mg/mL

Example of calculation of production rate:

Considering the case of ZB CdSe NCs, the flowrates and precursor concentrations conditions used in this paper lead to a CdSe concentrations in the final solution almost constant at ~ 3.75 $mg.mL^{-1}$, which corresponds to ~70% conversion. Therefore, the production rate will depends on the residence time needed to grow up the CdSe QDs. As a matter of fact, the flowrate required to produce a certain size will depends on the residence time required to grow up this particular size. As mentioned previously, the flowrate (Q in $m^3.s^{-1}$) can be calculated as: $Q = (V/R_t)*(\rho_{cond}/\rho_{pump})$. Given that the current reactor as an internal volume of 1,27 mL (V) and that the hexane density at 10 MPa in the pump (ρ_{pump}) and in conditions (ρ_{cond}) are 665 and 434 $kg.m^{-3}$, respectively, and considering a residence time of 5s (R_t), the required flowrate is 983 $\mu L.min^{-1}$, *i.e.* 59 $mL.h^{-1}$. By multiplying this value by the weight concentration (3.75 $mg.mL^{-1}$), we can calculate a production rate of ~ 220 $mg.h^{-1}$. However, considering a required residence time of 50s, the production rate will drop to ~ 22 $mg.h^{-1}$. Therefore, small blue-green QDs, which do not require long residence time, will be easier to produce in large quantities.