JINST 19 P07014 (2024)

Water-based Quantum Dots Liquid Scintillator for Neutrino Physics

Outline

1. Quantum Dots
2. Optical measurements
3. Cosmic ray test
4. Next step

Water-based quantum dots liquid scintillator for particle physics

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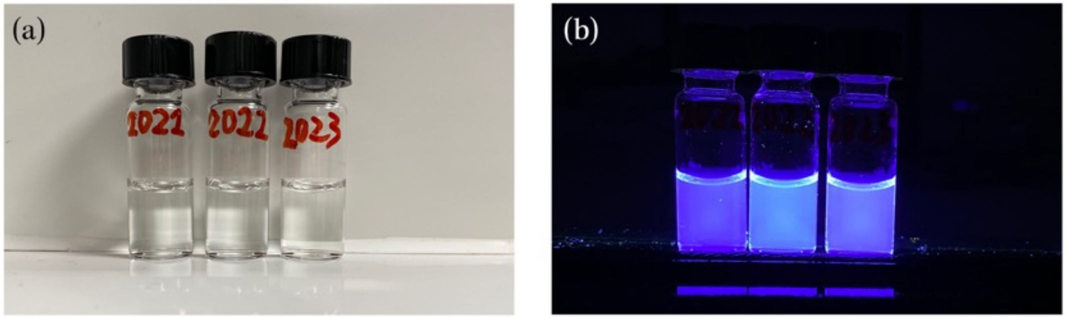

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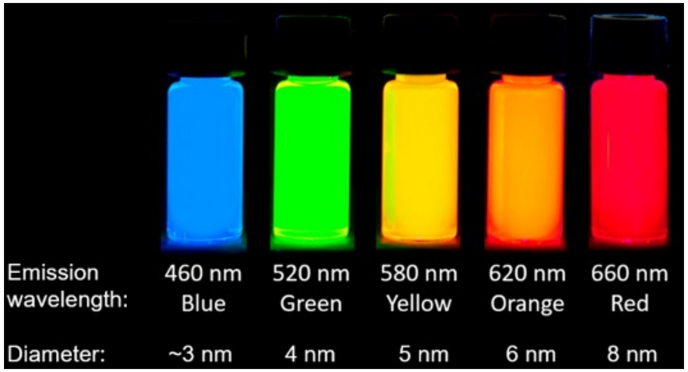
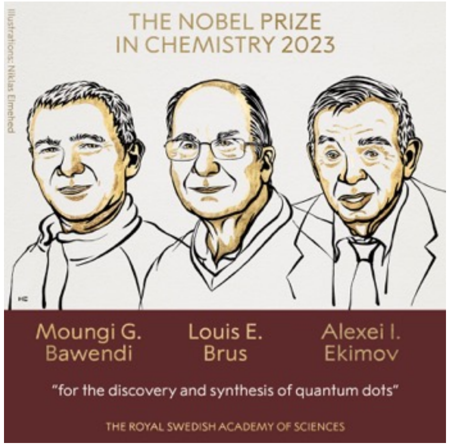
1. Quantum Dots

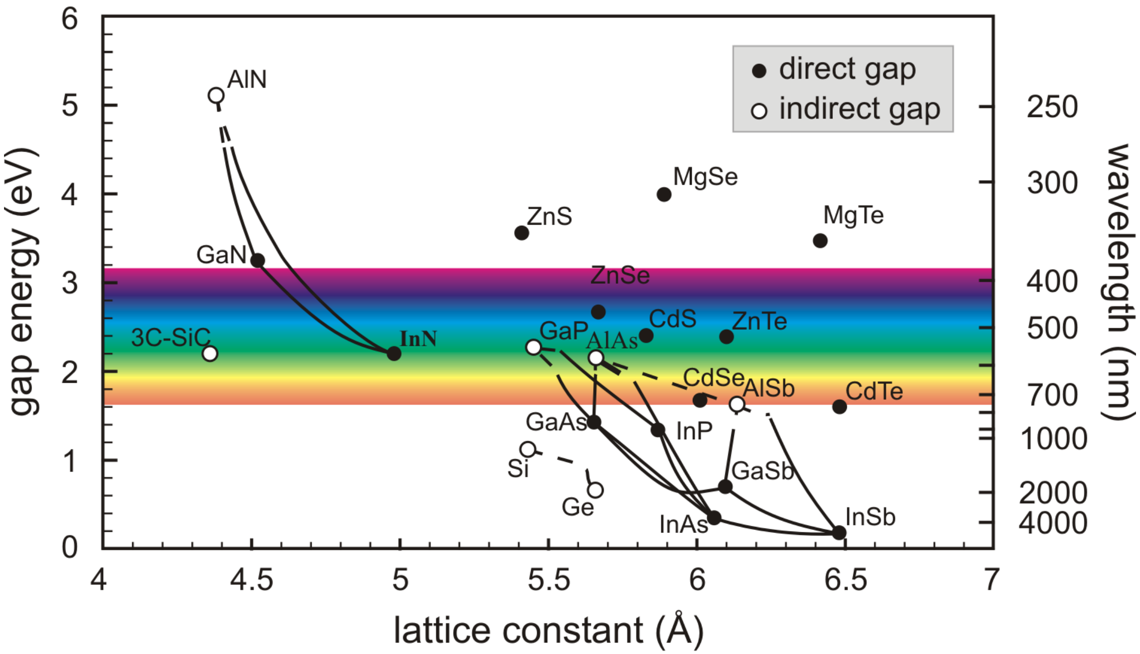
Semiconductor nano-particle
- Smaller than exciton radius (quantum confinement)
- ~2 – 10 nm, UV to infrared emission
- Tunable sharp emission spectrum
- Large category of choices (core type, size)
- High quantum yield (~50%)



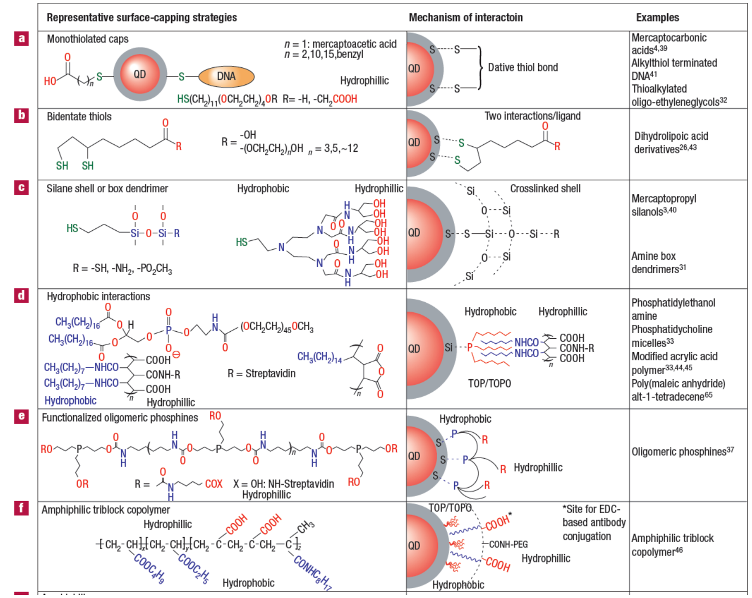
CdSe core QDs with CdS/ZnS shell
https://www.lateralflows.com/quantum-dots/



Noble prize in Chemistry (2023)



1. Quantum Dots

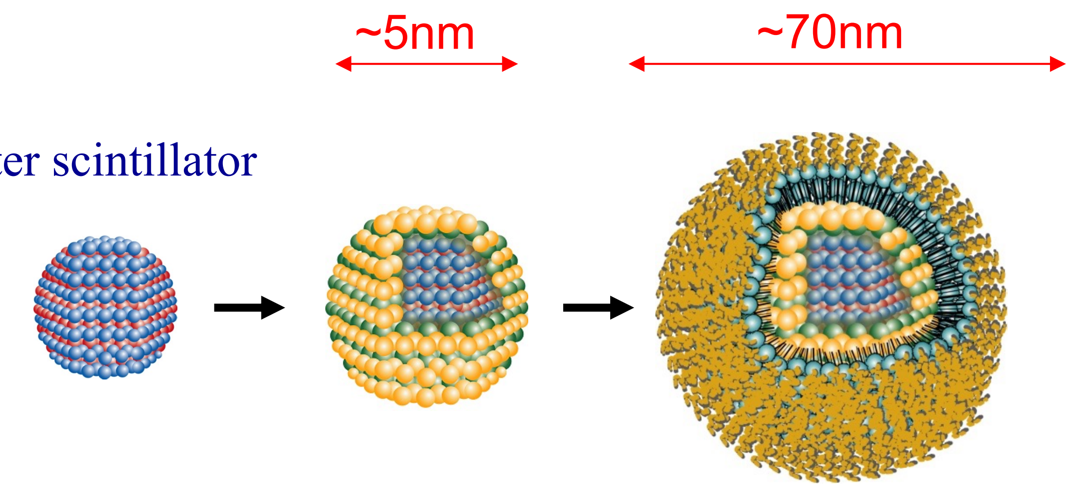


Semiconductor nano-particle

- Smaller than exciton radius (quantum confinement)
- ~2 – 10 nm, UV to infrared emission
- Tunable sharp emission spectrum
- Large category of choices (core type, size)
- High quantum yield (~50%)
- Surface layer engineering to change properties
  - Stability
  - Water solution

CdS-ZnS Quantum Dots-based water scintillator

1. High emission (QY ~ 50%) ✅
2. Stability (~ 3 yr) ✅
3. Emission (> 450nm) ⚠️
4. Environmental impact ❌
5. Affordable ❌



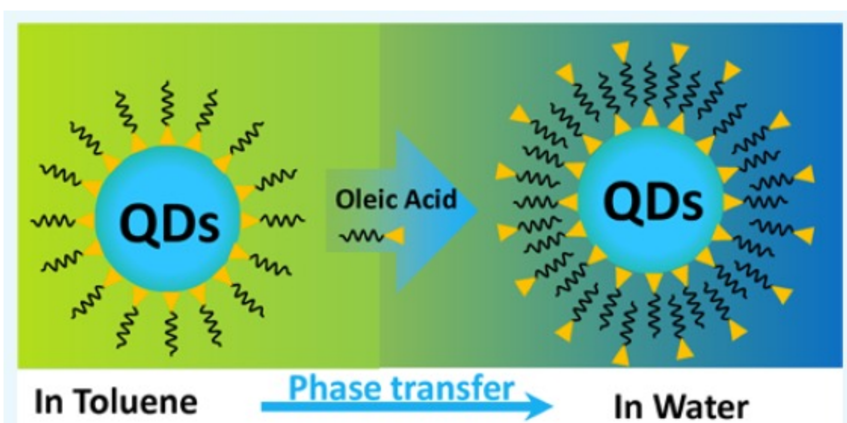
Quantum dot core (fragile) | QD with shell (stable) | QD with shell and ligand (colloid)

https://dx.doi.org/10.1021/acsomega.7b00316

1. Phase transfer

How to make water-based quantum dot solution

1. Dissolve CdS-ZnS QDs (10mg) in toluene
2. Evaporate toluene
3. Add hexane, sonic bath 1min
4. Add oleic acid
5. Add water
6. Sonic bath
7. Shake
8. Sonic bath, shake ... (1hr)
9. Leave in dark 24 hours

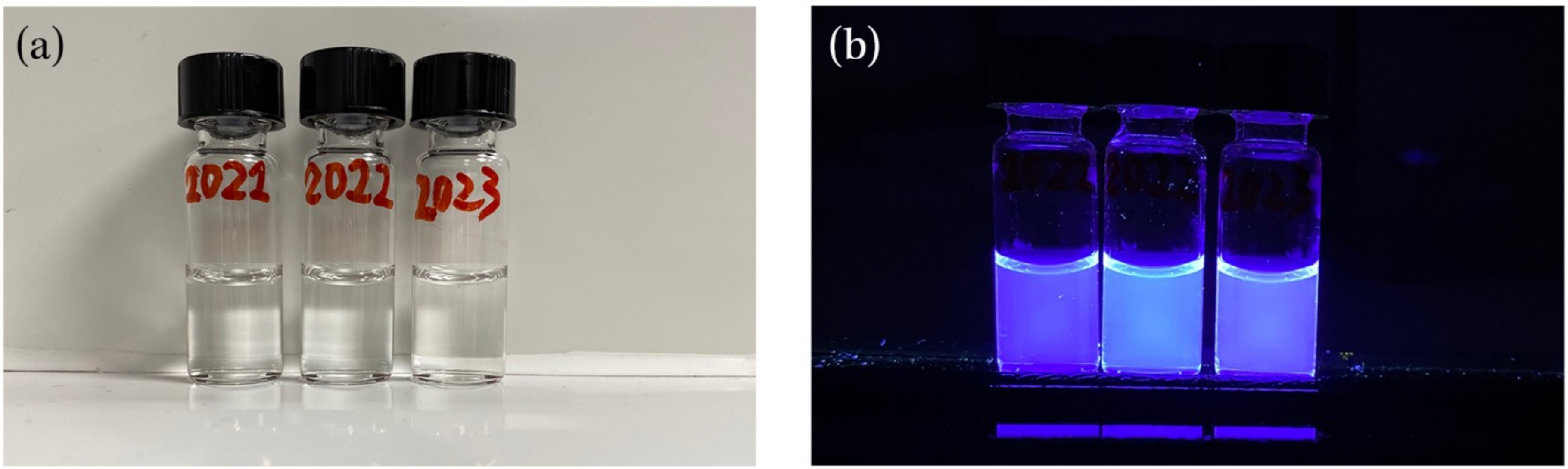


Chemistry is complicated

1. Water-based quantum dots liquid scintillator

We made 3 water-based QDs sample

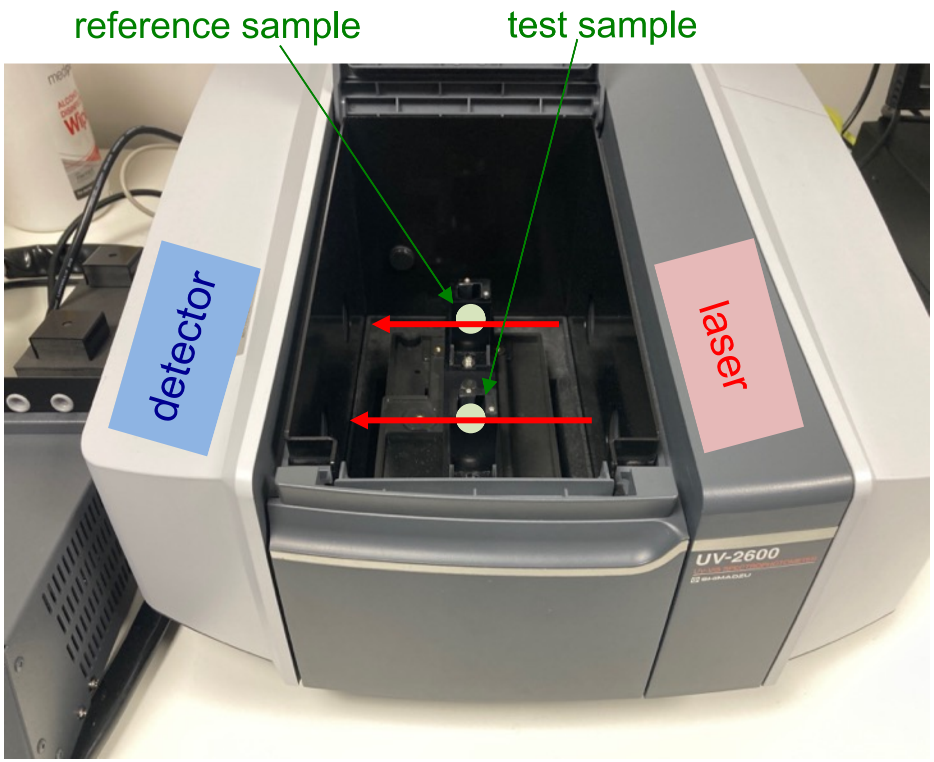
- Ageing tests
  - Quantum dots are stable over 3 years
  - No sign of agglomeration, but surface configuration is not stable
    → Need further study of phase transfer

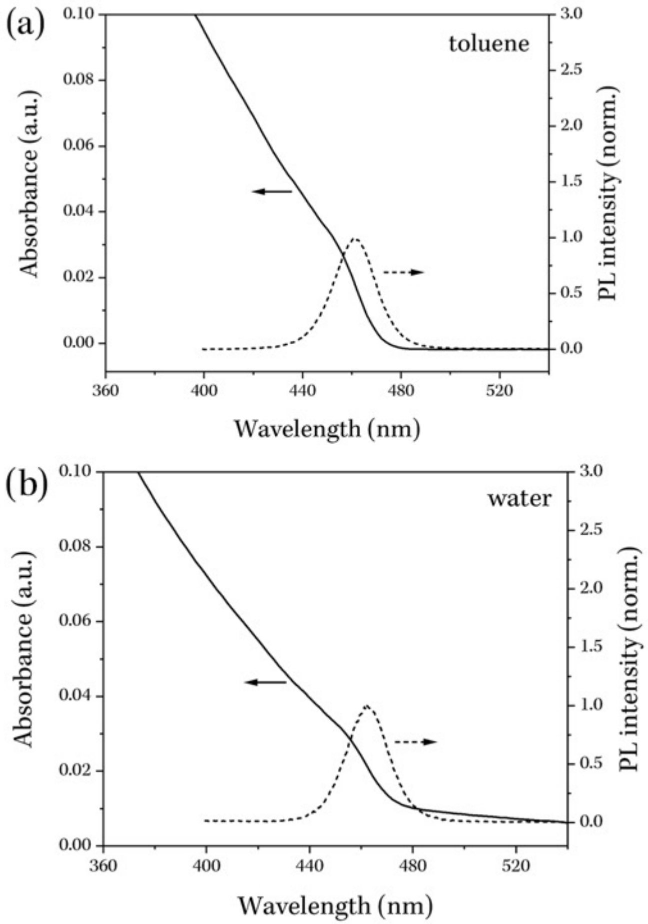


2. Absorbance measurement

Shimadzu UV-2600i spectrometer

- toluene QDs and water QDs show the same absorption peak (~460nm)
- No significance change of QD core by phase transfer

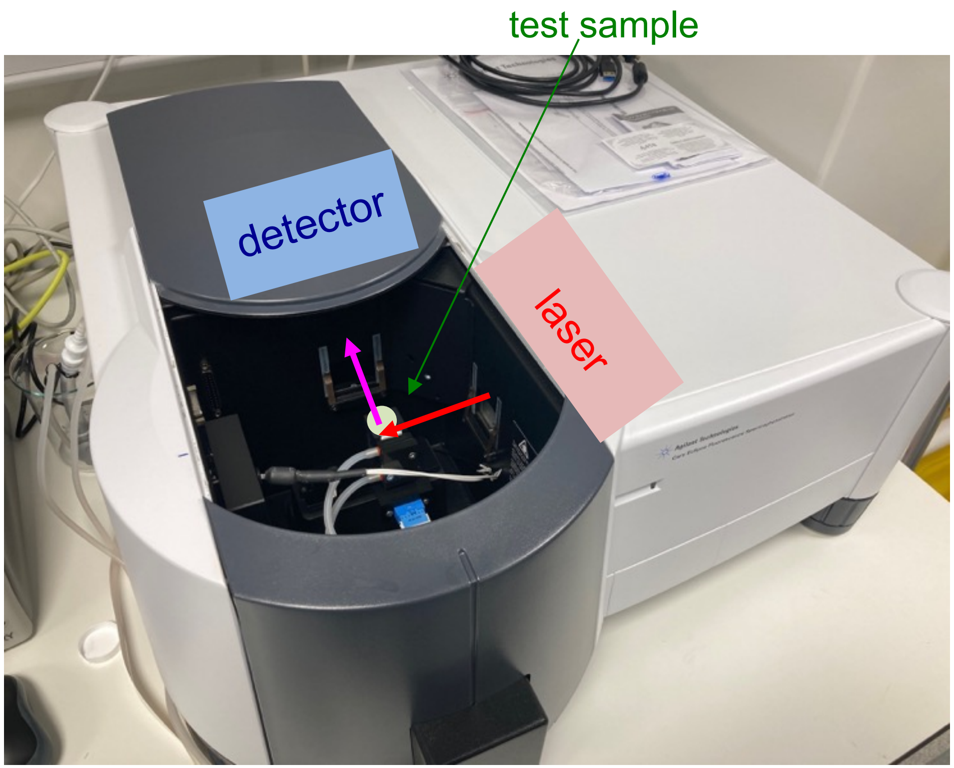


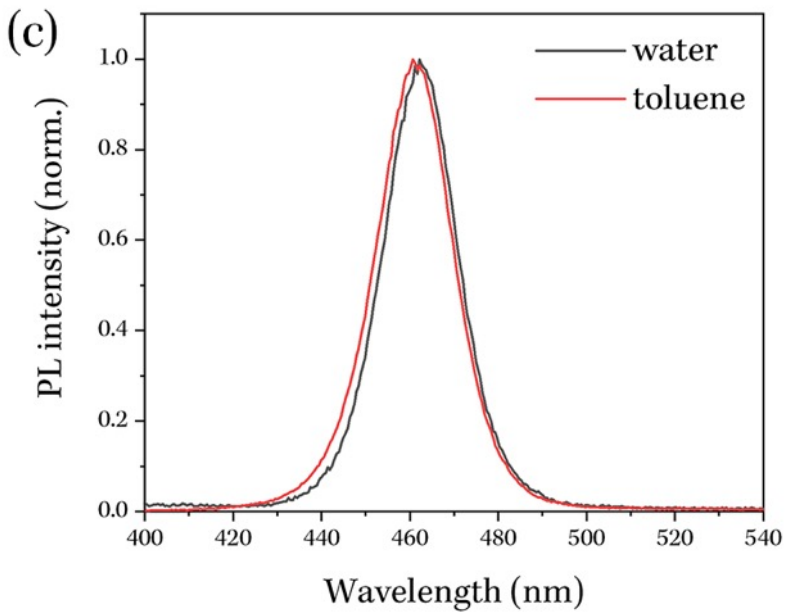


2. Fluorescence measurement

Agilent Technologies Cary Eclipse Fluorescence Spectrometer

- toluene QDs and water QDs show the same emission peak
- No significance change of QD core by phase transfer





2. Photoluminescence quantum yield (PLQY)

Measure absorbance and flourescence with different concentrations

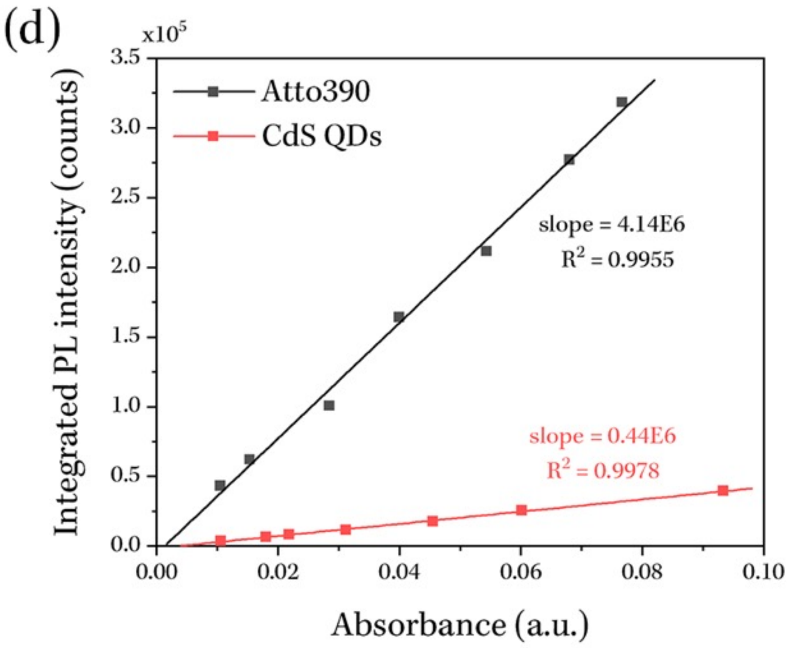
- Integrated PL intensity is a linear function of absorbance. Both integrated PL intensity and absorbance are measured with different concentration of the sample

$$I(A) = I_o + K \cdot A$$

- Obtained slope “K” is compared with the reference dye Atto390

- Measured PLQY is lower than the company value (~50%) suggesting the phase transfer lose some PLQY

PLQY = 9.5±0.5%



2. Dynamic light scattering (DLS) measurement

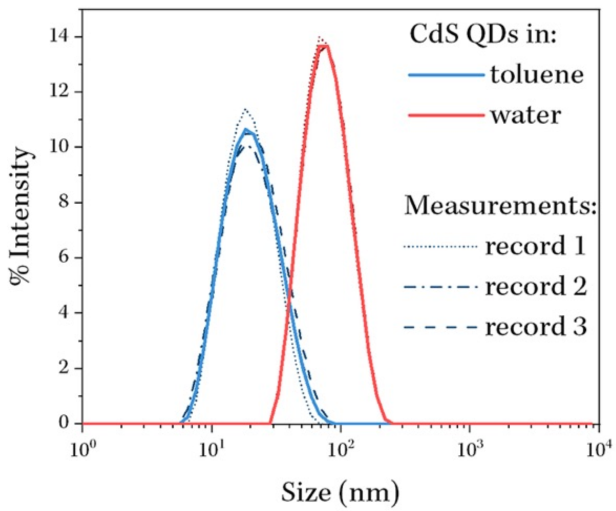
Malvern instruments Zetasizer Nano
- Measure the size of QDs from the back-scatted light
- Brownian motion gives time-dependent data

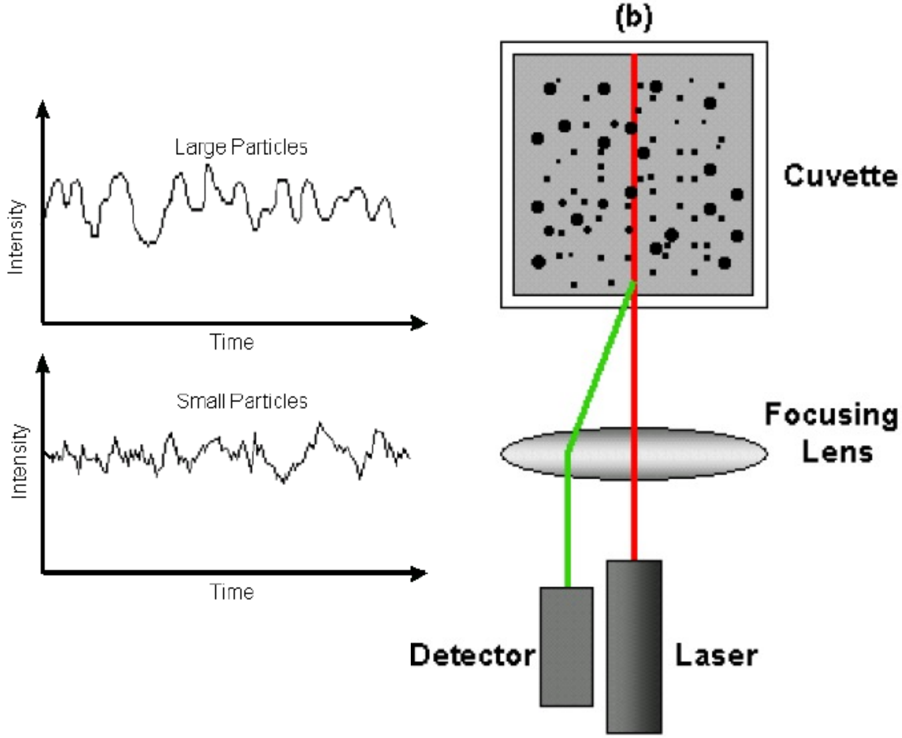
Hydrodynamic diameter d_H

$$D_H = \frac{k_B T}{3\pi\eta D}$$

$D_H^{Toluene} = 25 \pm 9$ nm
$D_H^{Water} = 71.6 \pm 0.3$ nm

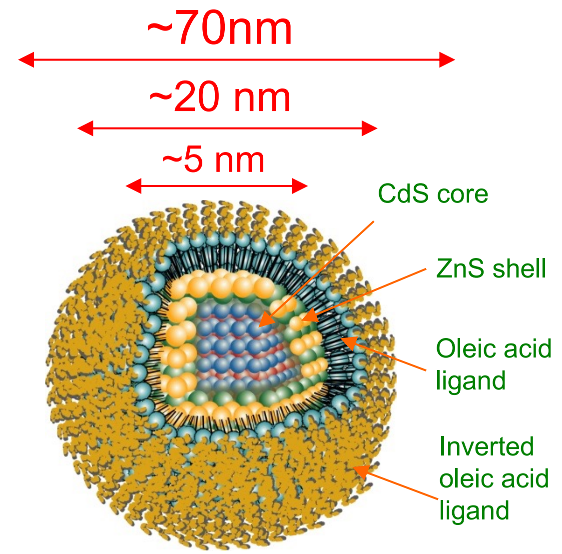
(b)





https://www.malvernpanalytical.com/en/products/technology/light-scattering/dynamic-light-scattering

2. Transmission electron microscope (TEM)



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Hydrodynamic diameter d_H

$$D_H = \frac{k_B T}{3\pi\eta D}$$

$D_H^{Toluene} = 25 \pm 9$ nm

$D_H^{Water} = 71.6 \pm 0.3$ nm

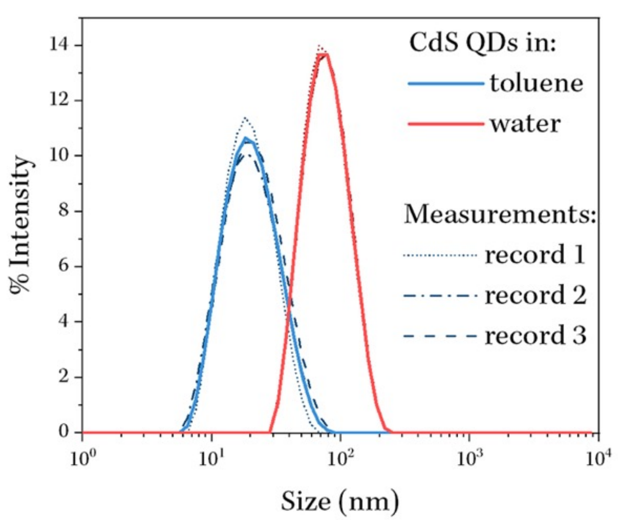
QD size is measured by TEM

- SEM, AFM, didn't work well

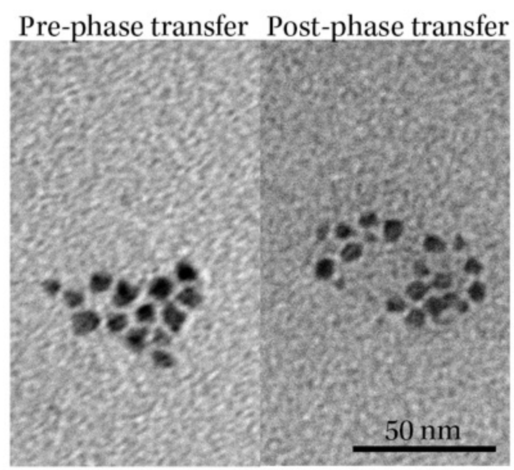
$D_{TEM}^{Toluene} = 6.4 \pm 1.0$ nm

$D_{TEM}^{Water} = 6,4 \pm 1.2$ nm

(b)



(d)

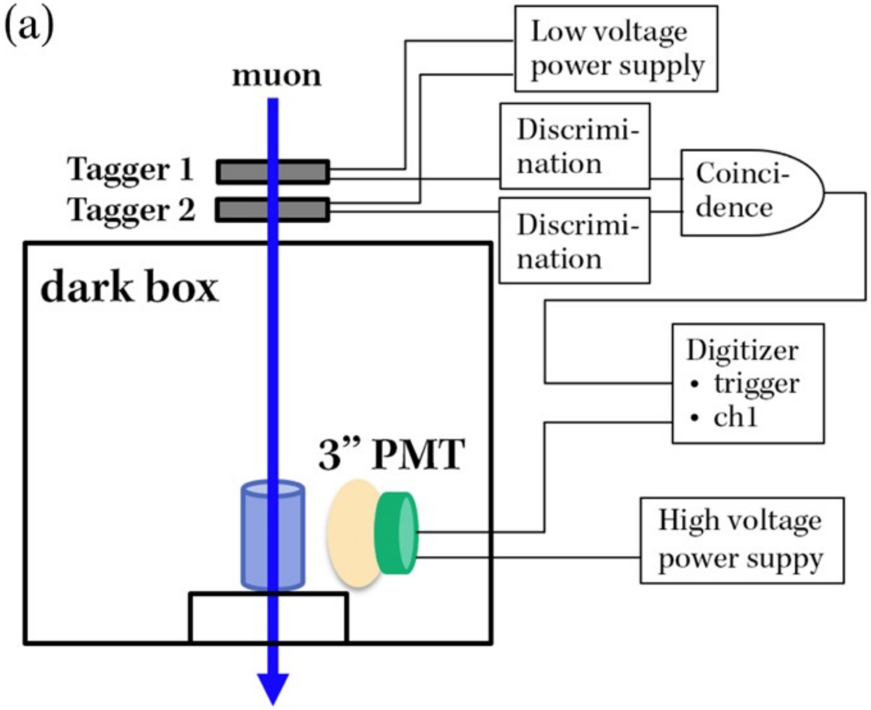


3. Cosmic ray test

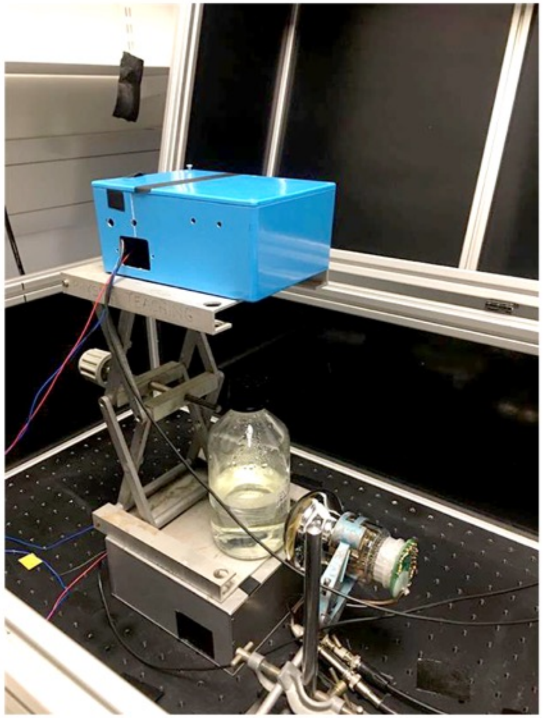
Set up

- Cosmic ray triggers (plastic scintillator + SiPM)
- 3-inch NNVT PMT
- CAEN 250MS/s digitizer

(a)



(b)



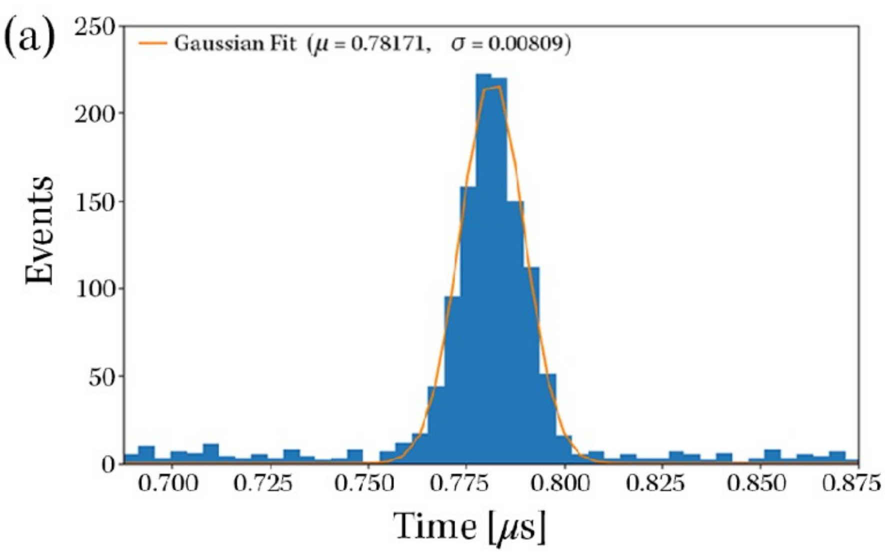
3. Cosmic ray test

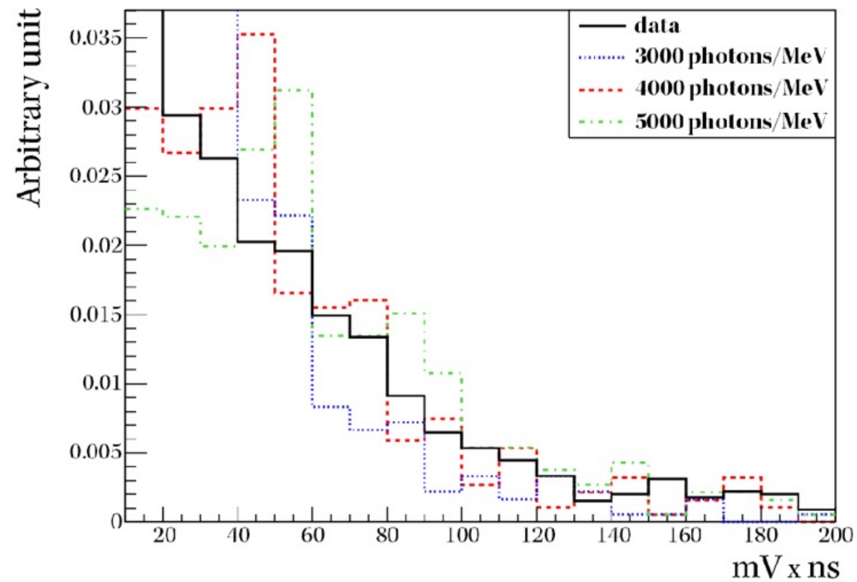
Timing data

- Quantum dots decay time is around 5ns
- Too fast to measure by 250MS/s (4ns bin) digitizer ($\tau < 8$ns)

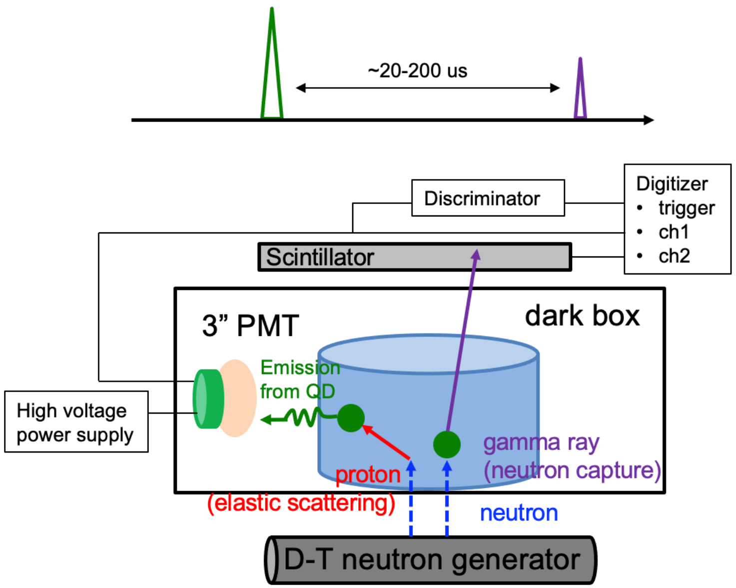
Charge data

- Data seems to have several 1000s photons / MeV
- Comparable emission strength with modern organic scintillator





4. Next step

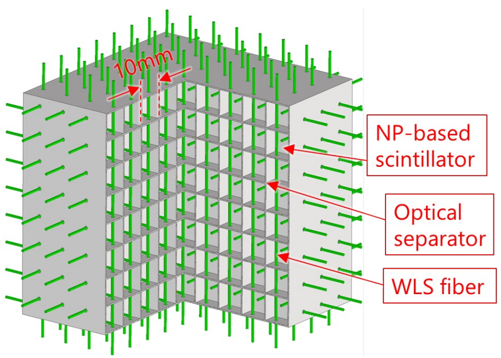


Nanocrystal water liquid scintillator works, but...

- 1L WbQDLS~£3k → ~£3M for 1 ton detector
- water is safe, but many nanocrystal is not safe

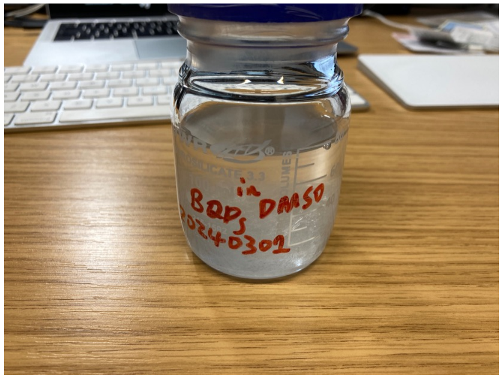
Future: Sustainable nanocrystal water scintillator

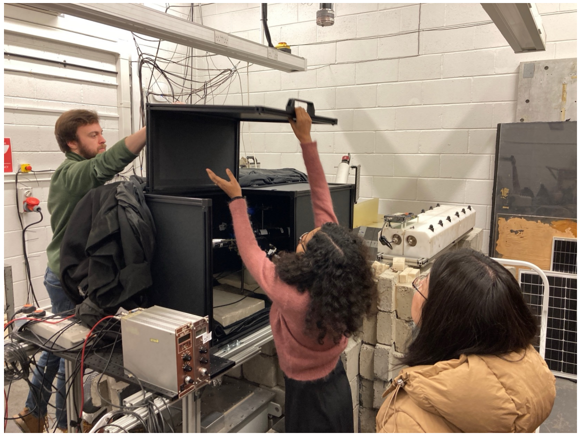
- no heavy metal: cheap, safe
- environment-friendly: green synthesis, recyclable
- neutron PID ability



Water-based liquid scintillator for Hyper-Kamiokande new new near detector (Kikawa, Kyoto)

Boron QD sample





QD neutron capture test (Sheffield fast pulse D-T gun)

5. Conclusions

Water-based liquid scintillator is successful made using CdS-ZnS quantum dots.

Water QDs photoluminescence quantum yield is 9.5±0.5%, lower than the company value (~50%).

Hydrodynamic diameter is measured by DLS, and water QDs (~70nm) is larger than toluene QDs (~20nm) as expected.

Scintillation response is measured from cosmic muons. Time constant seems very fast as expected (<8ns), and charge response suggests photon yield is comparable as typical organic liquid scintillators.

Sustainable nanocrystal water scintillator is the next step.

Thank you for your attention!

Backup

1. Quantum Dots

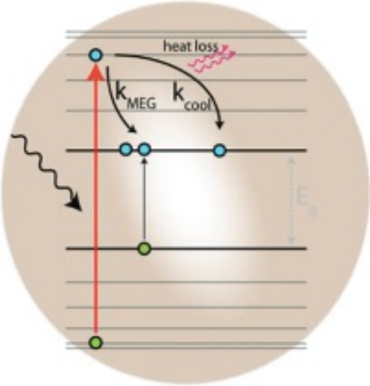
Display
- Tunable, sharp emission

Solar cell
- Multiple exciton generation

Biometric marker
- Water soluble
- Infrared
- Single molecular tracking

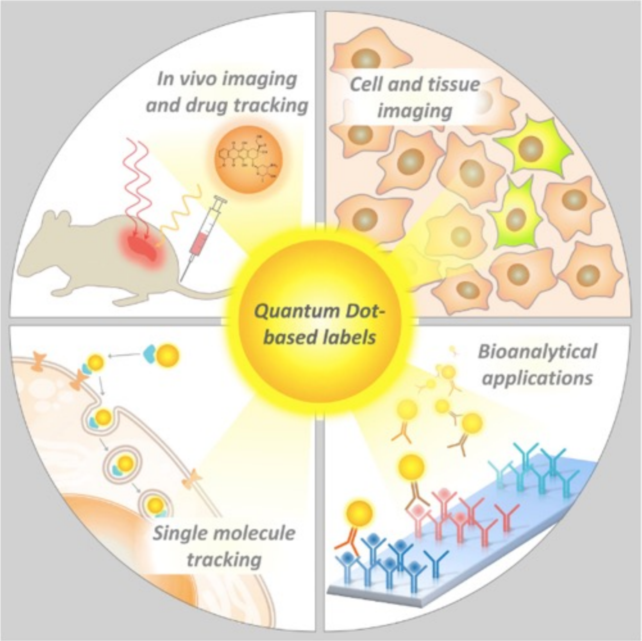
Quantum computer
- Spin qubit quantum computer

etc



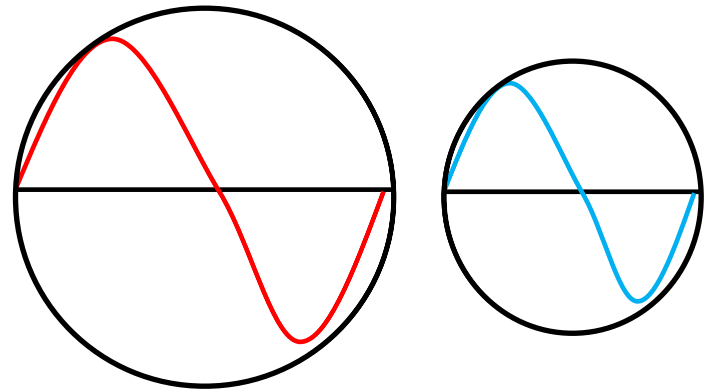
Energ. Environ. Sci. 13 (2020) 1347

Samsung QLED smart TV



ChemBioChem 17 (2016) 2103

1. Brus equation



Masses

- electron mass, m_e
- effective electron mass, ~$0.1m_e$ (CdSe)
- effective hole mass, ~$0.45m_e$
- effective exciton mass, μ ~$0.08m_e$

Size

- Exciton radius r ~6 nm

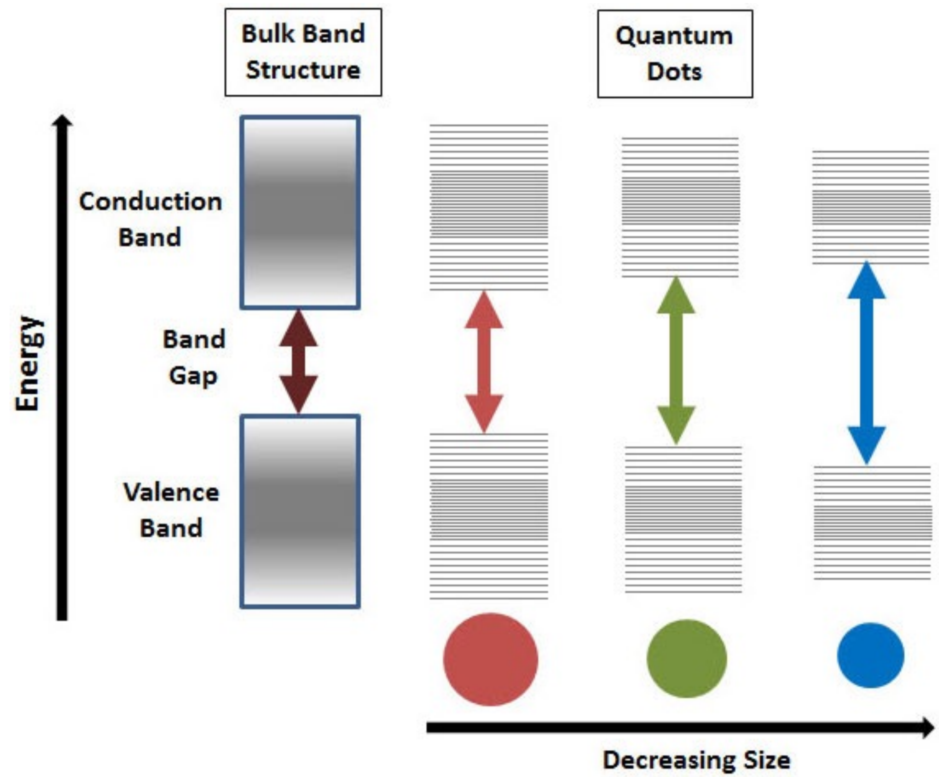
Exciton diameter 2r ~12 nm

- Quantum dots diameter: 2-10 nm

Band gap (Brus equation)

$$E_{QD} = E_{gap} + \frac{\hbar^2\pi^2}{2r^2\mu}$$

- Band gap is wider in quantum dots
- Quantum confinement



2. Fluorescence measurement

Agilent Technologies Cary Eclipse Fluorescence Spectrometer
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Photoluminescence quantum yield (PLQY)

$$I(A) = I_o + K \cdot A$$

- Integrated PL intensity is a linear function of absorbance. Both integrated PL intensity and absorbance are measured with different concentration of the sample
- Obtained slope "K" is compared with the reference dye Atto390
- Measured PLQY is lower than the company value (~50%) suggesting the phase transfer lose some PLQY

PLQY = 9.5±0.5%

Extinction peak

$$A(\lambda) = A_0 + A_{max} \cdot exp\left[-0.5\left(\frac{\lambda - \lambda_c}{w}\right)^2\right]$$

Empirical law with extinction peak
- mean QD diameter D

$D_{Empirical}$ = 5.22±0.01 nm
- concentration C

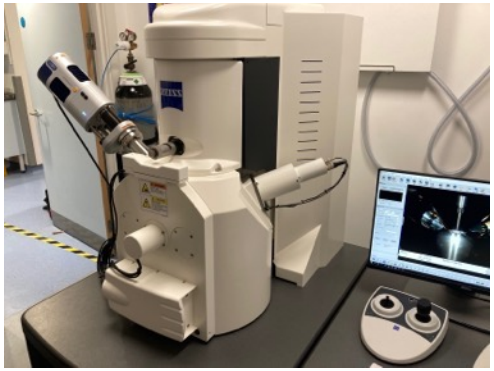
C = 42±1 nM

Typical organic scintillator (20% PPO)
- concentration ~ 4-30 mM
- cross-section area ~ 0.5-1nm^2

2. SEM, AFM, TEM

Scanning electron microscope (SEM)

- Sample is dried
- Gold is vacuum evaporated to make it conductive
- Not sensitive to QD size (~20nm)



Scanning electron microscope (SEM)

Atomic force microscope (AFM)

- Sample is dried
- Not sensitive to X-Y because of large tip
- Z measurement may be good?

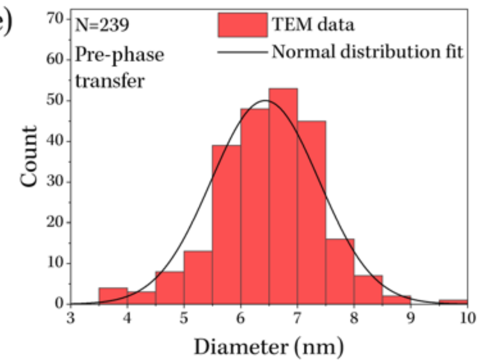
Atomic force microscope (AFM)

Transmission electron microscope (TEM)

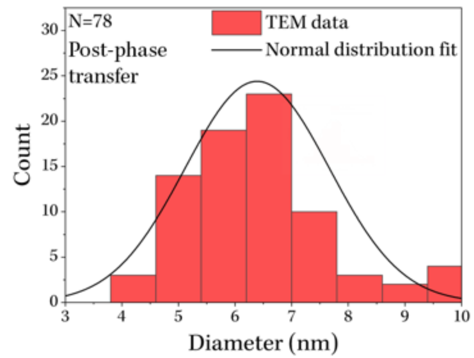
$D_{TEM}^{Toluene} = 6.4 \pm 1.0$ nm

$D_{TEM}^{Water} = 6,4 \pm 1.2$ nm

(e)



(f)



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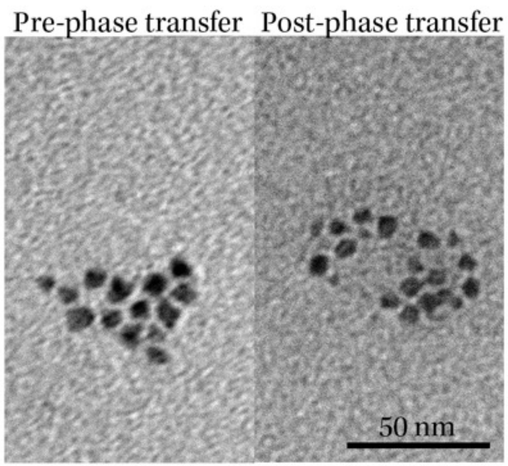

TEM image

KING'S College LONDON

2. Ageing

Sample		PLQY (%)	D_h (nm)	ζ (mV)
2021 WbQD	as prepared	15.6 ± 1.2	52.2 ± 0.3	not available
	in 2023	8.8 ± 0.8	48.7 ± 0.1	−13.8 ± 0.8
2022 WbQD	as prepared	8.8 ± 1.5	60 ± 1	−24 ± 2
	in 2023	14.5 ± 0.7	55.7 ± 0.3	−47 ± 2
2023 WbQD	as prepared	9.5 ± 0.5	71.6 ± 0.3	−24.6 ± 0.7

Absorbance and fluorescence

- No change over the period of 3 years

Size

- Slight decrease of the size (a few nm)
- Likely not losing layers, but re-organization of surface structure
- Zeta potential (surface charge) is changing over time, supporting this interpretation
- No sign of agglomeration

Photoluminescence quantum yield (PLQY)

- Large sample variation makes difficult to conclude

It seems water QDs are stable, but without ageing information of PLQY it's hard to say if they are suitable for particle detectors (~several years operation)

3. Cosmic ray test

Timing data
- Quantum dots decay time is around 5ns
- Too fast to measure by 250MS/s (4ns bin) digitizer (τ < 8ns)

Charge data
- Need simulation to extract information