Electronic supplementary information

Ultrabright dye-loaded spherical polyelectrolyte brushes and their fundamental structure-fluorescence tuning principles

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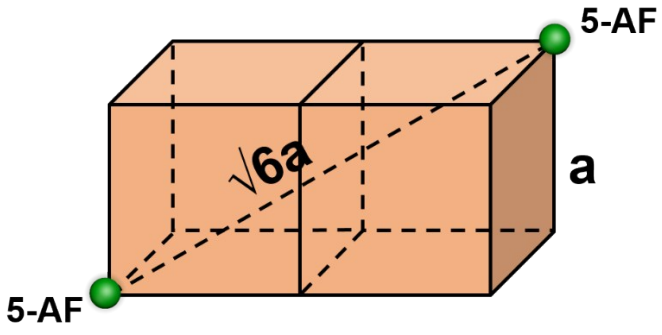

Figure S1. Hypothesized model of two adjacent immobilized 5-AF molecules on brushes.

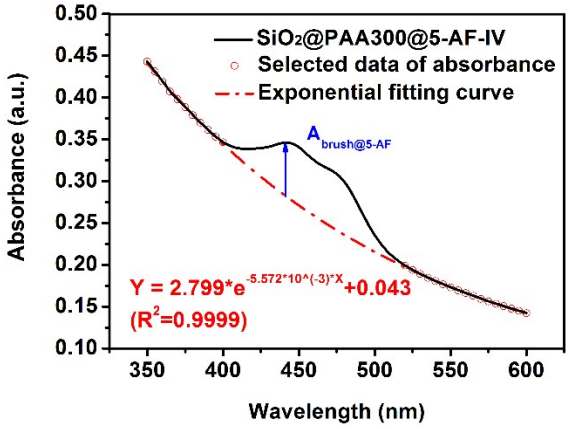

Figure S2. UV-vis spectrum of SiO_2@PAA300@5-AF-IV measured in water (black solid line). The scattering background of brush particle is identified by exponential fitting curve (red dash line) using data of absorbance measured at selected wavelengths (red circle points).

Calculations of QY:

For UV-vis measurement, when $\lambda = 430$ nm,

$absorbance_{R6G} = 0.036$,

$absorbance_{5\text{-}AF} = 0.029$,

corrective $absorbance_{SiO_2@PAA300@5\text{-}AF\text{-}IV} = absorbance_{SiO_2@PAA300@5\text{-}AF\text{-}IV} -$

$absorbance_{fitting} = 0.341 - 0.298 = 0.043$

For fluorescence measurement, when $\lambda_{excitation} = 430$ nm,

$emission\ integral_{R6G} = 8728.750$,

$emission\ integral_{5\text{-}AF} = 84.734$,

$emission\ integral_{SiO_2@PAA300@5\text{-}AF\text{-}IV} = 2136.854$

$$QY_{5\text{-}AF} = QY_{R6G} \times absorbance_{R6G}/absorbance_{5\text{-}AF} \times emission\ integral_{5\text{-}AF}/emission\ integral_{R6G} \times refraction\ index_{H_2O}^2/refraction\ index_{C_2H_5OH}^2$$

$$= 0.95 \times 0.036/0.029 \times 84.734/8728.750 \times 1.33^2/1.37^2$$

$$= 0.011$$

$QY_{SiO_2@PAA300@5\text{-}AF\text{-}IV} = QY_{R6G} \times absorbance_{R6G}/corrective\ absorbance_{SiO_2@PAA300@5\text{-}AF\text{-}IV}$
$\times\ emission\ integral_{SiO_2@PAA300@5\text{-}AF\text{-}IV}/emission\ integral_{R6G}$
$\times\ refraction\ index_{H_2O}^2/refraction\ index_{C_2H_5OH}^2$

$= 0.95 \times 0.036/0.043 \times 2136.854/8728.750 \times 1.33^2/1.37^2$

$= 0.184$

Calculations of brightness:

Number of 5-AF molecules on per SiO_2@PAA300@5-AF-IV
= (loading amount of 5-AF on 1 mg brush) / (particle number of 1 mg brush)
= (0.062 ± 0.003 μmol/mg brush $\times N_A \times$ 1 mg) / $((1.505 \pm 0.213)\times10^{11})$

= $((0.062 \pm 0.003)\times10^{-6}$ mol/mg brush $\times 6.02\times10^{23}$/mol $\times$ 1 mg) / $((1.505 \pm 0.213)\times10^{11})$

= $(2.48 \pm 0.37)\times10^5$

According to the QY results, a 5-AF molecule brightness on SiO_2@PAA300@5-AF-IV
= $QY_{5\text{-}AF\ on\ brush}$ / QY_{R6G} × a R6G molecule brightness
= $(0.180 \pm 0.021)/0.95$ × a R6G molecule brightness
= (0.189 ± 0.022) × a R6G molecule brightness
Therefore, $(2.48 \pm 0.37)\times10^5$ 5-AF molecules on per SiO_2@PAA300@5-AF-IV is equal to the brightness of $(2.48 \pm 0.37)\times10^5 \times(0.189 \pm 0.022) = (4.70 \pm 0.89)\times10^4$ molecules of R6G.

As the brightness of a single CdSe/ZnS QD is equal to 20 times brightness of a single R6G molecule according to related references,[1-4] then a fluorescent brush particle of SiO_2@PAA300@5-AF-IV is calculated to be $(4.70 \pm 0.89)\times10^4/20$ = **2350 ± 445 times** brighter than a single QD.

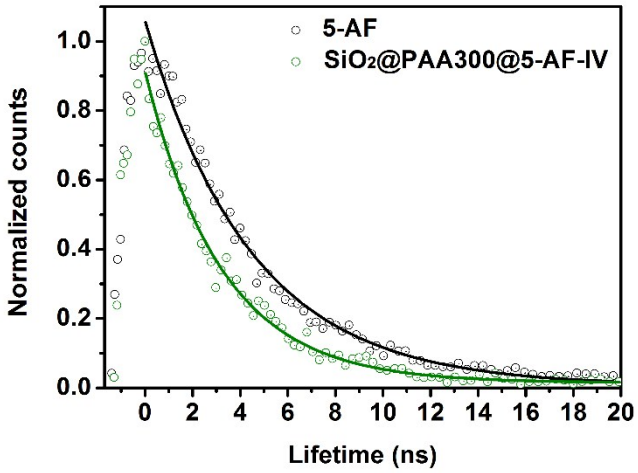

Figure S3. Fluorescent lifetime curves of 5-AF and SiO_2@PAA300@5-AF-IV.

References

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3 W. C. Chan, D. J. Maxwell, X. Gao, R. E. Bailey, M. Han and S. Nie, *Current opinion in biotechnology*, 2002, **13**, 40-46.S4

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