**Electronic Supplementary Information (ESI) for** 

## Synthesis and Aggregation Properties of A Series of Dumbbell

## Polyhedral-Oligosilsesquioxane-Perylene Diimide Triad

Ying Zhang, Liangliang Zhang, Heyuan Liu, Di Sun, and Xiyou Li\*



Fig. S1 UV-vis absorption (left) and fluorescence (right) spectra of 2a-c (a) and 3a-c

(b) in chloroform  $(5.0 \times 10^{-6} \text{M})$  at room temperature.





Fig. S2 Normalized Fluorescence spectra of thin films of 2a-c (a) and 3a-c (b).

(1): With monomeric **3a**  $(5.0 \times 10^{-6} \text{M})$  as reference.



Fig. S3 The X-ray diffraction patterns of thin film of compound 1a-c, 2a-c and 3a-c on quartz glass substrate

## Single Crystal X-ray Analysis

1b	3b	3c
$C_{86}H_{146}N_2O_{28}Si_{16}$	C132H190N2O32Si16 <sup>-2</sup> CHCl3	C132H190N2O32Si163CHCl3
2105.49	2937.00	3124.40
triclinic	triclinic	triclinic
<i>p-1</i>	<i>p-1</i>	<i>p-1</i>
11.3824(2)	10.975(4)	15.310(8)
21.8344(4)	21.227(7)	15.323(9)
23.7734(5)	34.042(10)	37.78(2)
86.5313(16)	87.099(7)	100.751(10)
81.6042(18)	82.157(6)	95.049(11)
83.2088(17)	83.536(6)	102.622(10)
5798.4(2)	7802(4)	8420(8)
2	2	2
1.206	1.250	1.232
293	196	190
1.5418	0.71073	0.71073
2700	3120	3300
2.215	0.300	0.328
0.1186	0.1484	0.1417
60760	38909	41600
21454	27089	29191
21454/608/1109	27089/885/1641	29191/837/1516
$R_1 = 0.2148$ ,	$R_1 = 0.1564,$	$R_1 = 0.1858,$
$wR_2 = 0.5006$	w <i>R</i> <sub>2</sub> =0.3681	w <i>R</i> <sub>2</sub> =0.4245
$R_1 = 0.3009,$	$R_1 = 0.4307$ ,	$R_1=0.4064,$
$wR_2 = 0.5282$	$wR_2 = 0.4660$	wR <sub>2</sub> =0.5002
1.159	0.778	0.864
	1b $C_{86}H_{146}N_2O_{28}Si_{16}$ $2105.49$ triclinic $p$ - $l$ $11.3824(2)$ $21.8344(4)$ $23.7734(5)$ $86.5313(16)$ $81.6042(18)$ $83.2088(17)$ $5798.4(2)$ $2$ $1.206$ $293$ $1.5418$ $2700$ $2.215$ $0.1186$ $60760$ $21454$ $21454/608/1109$ $R_1$ = $0.2148$ , $wR_2$ = $0.5006$ $R_1$ = $0.3009$ , $wR_2$ = $0.5282$ $1.159$	1b $3b$ $C_{86}H_{146}N_2O_{28}Si_{16}$ $C_{132}H_{190}N_2O_{32}Si_{16}2CHCl_3$ $2105.49$ $2937.00$ triclinictriclinic $p$ -l $p$ -l $11.3824(2)$ $10.975(4)$ $21.8344(4)$ $21.227(7)$ $23.7734(5)$ $34.042(10)$ $86.5313(16)$ $87.099(7)$ $81.6042(18)$ $82.157(6)$ $83.2088(17)$ $83.536(6)$ $5798.4(2)$ $7802(4)$ $2$ $2$ $1.206$ $1.250$ $293$ $196$ $1.5418$ $0.71073$ $2700$ $3120$ $2.215$ $0.300$ $0.1186$ $0.1484$ $60760$ $38909$ $21454$ $27089/885/1641$ $R_1=0.2148,$ $R_1=0.1564,$ $wR_2=0.5006$ $wR_2=0.3681$ $R_1=0.3009,$ $R_1=0.4307,$ $wR_2=0.5282$ $wR_2=0.4660$ $1.159$ $0.778$

 Table 1 Crystal data and structure refinements for 1b, 3b and 3c.