Electronic Supplementary Material (ESI) for RSC Advances.


**Supporting Information**

# Hybrid silicon-carbon nanostructures for broadband optical absorption

Wen-Hua Yang, [*,a] Wen-Cai Lu, [*,ab]

[a]College of Physics and Laboratory of Fiber Materials and Modern Textile, Growing Base for State Key Laboratory, Qingdao University, Qingdao, Shandong 266071, P. R. China

[b]Institute of Theoretical Chemistry, Jilin University, Changchun, Jilin 130021, P. R. China

K. M. Ho[c] and C. Z. Wang[c]

[c]Ames Laboratory-U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, IA 50011, U.S.A

**Table S1 HOMO-LUMO gap and binding energy of $Si_m$ (m=7-13) cluster,**

| | Gap (eV) | | $E_b$ (eV) |
|---|---|---|---|
| | This work | Ref 1 | |
| $Si_7$ | 3.178 | 3.157 | 4.287 |
| $Si_8$ | 2.595 | 2.575 | 4.207 |
| $Si_9$ | 2.920 | 2.930 | 4.286 |
| $Si_{9\text{-}A}$ | 1.706 | 1.706 | 4.208 |
| $Si_{10}$ | 3.034 | 3.046 | 4.359 |
| $Si_{11}$ | 2.798 | 2.777 | 4.304 |
| $Si_{12\text{-}A}$ | 2.757 | 2.757 | 4.138 |
| $Si_{13}$ | 1.766 | 1.811 | 4.286 |

1 W. Qin, W. C. Lu, L. Z. Zhao, Q. J. Zang, C. Z. Wang, K. M. Ho, *J. Phys.: Condens. Matter.,* 2009, **21**, 455501

**Table S2 Excitation energies and oscillator strengths ( $f$ ) for major transitions of $Si_m$ (m=7-13)**

| | Excitation energy (eV/nm) | $f$ | Major transitions and weight | |
|---|---|---|---|---|
| $Si_7$ | 8.14/152.38 | 2.3016 | H-7→L+3 | 50.07% |
| | 9.30/133.25 | 1.9894 | H-9→L+6 | 33.03% |
| | | | H-8→L+7 | 33.04% |
| | | | H-3→L+13 | -20.29% |
| | 9.97/124.40 | 3.6930 | H-9→L+1 | 22.87% |
| | | | H-8→L+2 | -22.87% |
| | | | H-6→L+9 | 21.82% |
| | | | H-5→L+10 | -21.82% |
| $Si_8$ | 7.91/156.67 | 1.6028 | H-8→L+8 | 22.76% |
| | | | H-3→L+7 | 44.49% |
| | 9.71/127.65 | 1.7168 | H-1→L+17 | 36.35% |
| | | | H-1→L+20 | 26.56% |
| $Si_9$ | 8.49/146.05 | 1.3009 | H-13→L+2 | -20.91% |
| | | | H-10→L+4 | 33.60% |
| | | | H-8→L+14 | -25.76% |
| | 9.50/130.44 | 1.3950 | H-12→L+6 | 28.40% |
| | | | H-10→L+7 | 28.87% |
| | | | H-9→L+12 | -26.72% |
| | | | H-8→L+16 | 22.68% |
| $Si_{10}$ | 6.90/179.75 | 0.2339 | H-6→L+14 | 66.50% |
| $Si_{11}$ | 7.29/169.99 | 0.4075 | H-6→L+12 | 60.97% |
| $Si_{13}$ | 6.17/200.73 | 0.1515 | H-13→L+2 | 45.54% |
| | | | H-10→L+8 | 31.58% |
| | | | H-6→L+15 | -23.33% |
| $Si_{9\text{-}A}$ | 8.98/138.00 | 2.1638 | H-7→L+13 | -20.10% |
| | | | H-3→L+9 | 37.13% |
| $Si_{12\text{-}A}$ | 6.20/200.08 | 0.2145 | H-13→L+3 | 36.32% |
| | | | H-12→L+2 | 37.08% |
| | | | H-3→L+20 | 22.73% |
| | | | H-2→L+19 | 22.79% |

*Major transitions are those contributing more than 20%. Assignment: H = HOMO, L = LUMO.

**Table S3 Excitation energies and oscillator strengths ( $f$ ) for major transitions of $Si_m@C_{2n}$ (m=7-13, 2n=60, 70, 76 and 84)**

| | Excitation energy (eV/nm) | $f$ | Major transitions and weight | |
|---|---|---|---|---|
| $Si_7@C_{60}$-$I_h$ | 3.76/329.88 | 0.0315 | H-1→L+14 | 30.99% |
| | | | H-1→L+15 | 34.51% |
| | 5.34/232.27 | 0.0416 | H-7→L+16 | 32.58% |
| | | | H-14→L+9 | -24.23% |
| | | | H-8→L+12 | -24.98% |
| | | | H-2→L+23 | 20.52% |
| $Si_7@C_{70}$-$D_{5h}$ | 3.12/397.34 | 0.0319 | H-4→L+11 | 40.46% |
| | | | H-2→L+12 | 22.01% |
| | | | H→L+16 | 21.64% |
| | | | H→L+17 | -25.98% |
| | 4.25/291.52 | 0.0255 | H-13→L+2 | -20.22% |
| | | | H-10→L+5 | 32.33% |
| | | | H-9→L+6 | 22.30% |
| | 4.33/286.61 | 0.0258 | H-12→L+3 | -28.60% |
| | | | H-9→L+7 | 32.10% |
| | | | H-1→L+22 | -23.86% |
| $Si_7@C_{76}$-$D_2$ | 4.05/306.31 | 0.0343 | H-11→L+5 | 27.17% |
| | | | H-8→L+11 | -20.17% |
| | | | H-7→L+10 | 26.94% |
| | | | H-5→L+19 | -21.93% |
| | 4.26/291.25 | 0.0272 | H-13→L+6 | 42.23% |
| | | | H-9→L+8 | 33.34% |
| $Si_7@C_{84}$-$D_2$ | 2.01/427.65 | 0.0255 | H-2→L+2 | 26.27% |
| | | | H→L+9 | 42.44% |
| | | | H→L+10 | 26.27% |
| | | | H→L+11 | 28.60% |
| | 2.90/427.65 | 0.0156 | H-9→L+1 | -24.34% |
| | | | H-8→L+1 | 32.59% |
| | | | H-8→L+2 | 24.33% |
| | | | H-2→L+9 | -23.67% |
| | 4.31/287.94 | 0.0208 | H-7→L+14 | 29.22% |

| | Excitation energy (eV/nm) | $f$ | Major transitions and weight | |
|---|---|---|---|---|
| $Si_8@C_{70}$-$D_{5h}$ | 2.24/554.6 | 0.0235 | H-5→L+2 | 49.42% |
| | | | H→L+8 | 29.34% |
| | 3.11/398.10 | 0.0452 | H-12→L H- | 22.61% |
| | | | 9→L+1 | 35.92% |
| | | | H-4→L+8 | 24.68% |
| | | | H→L+13 | 26.19% |
| | 4.51/274.81 | 0.025 | H-14→L+4 | 25.93% |
| | | | H-5→L+18 | 38.87% |
| $Si_8@C_{76}$-$D_2$ | 4.48/276.46 | 0.0222 | H-13→L+6 | 30.46% |
| $Si_8@C_{84}$-$D_2$ | 4.39/282.53 | 0.0251 | H-23→L | 24.89% |
| | | | H-22→L+2 | -24.55% |
| $Si_9@C_{70}$-$D_{5h}$ | 2.28/543.70 | 0.0194 | H-5→L | 29.71% |
| | | | H-4→L+3 | -21.11% |
| | | | H-4→L+5 | -23.09% |
| | 3.43/361.28 | 0.0518 | H-7→L+10 | -26.26% |
| | | | H-4→L+6 | 26.15% |
| | | | H-3→L+15 | -21.43% |
| | | | H-2→L+18 | 33.55% |
| | 4.54/272.96 | 0.0198 | H-13→L+4 | 29.31% |
| | | | H-10→L+6 | 32.06% |
| $Si_9@C_{76}$-$D_2$ | 4.11/301.81 | 0.0205 | H-15→L+1 | -21.93% |
| | | | H-13→L+6 | 28.61% |
| | | | H-7→L+14 | 20.46% |
| $Si_9@C_{84}$-$D_2$ | 4.33/286.65 | 0.0226 | H-12→L+12 | 27.90% |
| $Si_{10}@C_{70}$-$D_{5h}$ | 1.90/650.93 | 0.0322 | H-6→L+1 | -21.87% |
| | | | H-5→L | -21.91% |
| | 1.90/650.93 | 0.0322 | H-2→L+4 | -25.60% |
| | | | H-1→L+4 | 36.17% |
| $Si_{10}@C_{70}$-$D_{5h}$ | 3.13/396.17 | 0.0356 | H-10→L+4 | 28.94% |
| | | | H-9→L+8 | 27.84% |
| | | | H-5→L+12 | 33.29% |
| | | | H-1→L+16 | -22.93% |
| | 4.16/297.57 | 0.0307 | H-13→L+1 | 32.32% |

| | Excitation energy (eV/nm) | *f* | Major transitions and weight | |
|---|---|---|---|---|
| $Si_{10}@C_{70}$-$D_{5h}$ | 4.16/297.57 | 0.0307 | H-12→L+2 | 39.19% |
| $Si_{10}@C_{76}$-$D_2$ | 4.36/284.53 | 0.026 | H-16→L | 28.11% |
| | | | H-13→L+7 | -24.14% |
| | | | H-6→L+20 | -20.05% |
| | | | H-1→L+29 | 22.05% |
| $Si_{10}@C_{84}$-$D_2$ | 4.19/296.18 | 0.0204 | H-6→L+20 | 30.45% |
| $Si_{11}@C_{76}$-$D_2$ | 4.04/306.53 | 0.0403 | H-14→L+7 | 21.66% |
| | | | H-12→L+13 | 24.85% |
| | | | H-9→L+14 | -21.17% |
| $Si_{11}@C_{84}$-$D_2$ | 4.23/293.28 | 0.0165 | H-17→L+7 | 20.54% |
| | | | H-7→L+17 | 29.79% |
| | | | H-6→L+18 | -20.16% |
| | | | H-5→L+18 | -23.05% |
| $Si_{13}@C_{84}$-$D_2$ | 4.22/294.10 | 0.0132 | H-18→L+6 | -20.05% |
| | | | H-16→L+7 | 28.70% |
| $Si_{9\text{-}A}@C_{70}$-$D_{5h}$ | 2.24/552.69 | 0.0151 | H-1→L+9 | 45.93% |
| | | | H→L+10 | 28.15% |
| | 3.30/375.76 | 0.0314 | H-8→L+10 | 30.39% |
| | | | H-6→L+10 | 27.20% |
| | | | H-1→L+17 | -20.81% |
| | | | H→L+18 | -27.61% |
| | 4.33/286.29 | 0.0212 | H-11→L+5 | 23.01% |
| | | | H-4→L+19 | 26.68% |
| | | | H-3→L+19 | 23.09% |
| $Si_{12\text{-}A}@C_{84}$-$D_2$ | 4.16/298.29 | 0.016 | H-18→L+6 | 30.08% |
| | | | H-17→L+8 | -26.36% |
| | | | H-10→L+12 | -20.46% |

*Major transitions are those contributing more than 20%. Assignment: H = HOMO, L = LUMO.