**Supplementary Information:**

**Structural Transition of Nanogel Star Polymers with pH by Controlling PEGMA Interactions with Acid or Base Copolymers**

Lisa E. Felberg1\*, Anjali Doshi3\*, Greg L. Hura5, Joseph Sly6, Victoria A. Piunova6, Robert Miller6, Julia E. Rice6, William C. Swope6, Teresa Head-Gordon1-5§

*1Department of Chemical and Biomolecular Engineering, 2Department of Chemistry, 3Department of Bioengineering, University of California Berkeley, Berkeley, California 94720, USA*

 *4Chemical Sciences Division and 5Physical Biosciences Division, Lawrence Berkeley National Labs, Berkeley, California 94720, USA*

*6IBM Research, IBM Almaden Research Center, San Jose, California 95120, USA*

**Table S1. The form factor and fitting parameters for DVB-PS-PEGMA series.** The Guinier region was fit to Q\*I(Q) < 1.3.

|  |  |  |  |
| --- | --- | --- | --- |
| **Form Factor** | **Guinier** | **Star Polymer** | **Fit** |
| **pH** | **Rg (Å)** | α | **ξ (Å)** | χ2**/Npts** |
| 2.76 | 80.98 | 2.19 | 12.09 | 0.95 |
| 2.78 | 82.33 | 1.99 | 11.26 | 0.94 |
| 2.85 | 78.45 | 1.98 | 11.47 | 0.38 |
| 3.18 | 79.31 | 2.11 | 11.75 | 0.38 |
| 7.06 | 78.50 | 1.95 | 11.23 | 0.49 |
| 8.32 | 82.47 | 2.06 | 11.38 | 0.97 |
| 8.44 | 77.21 | 2.01 | 11.55 | 0.78 |
| 8.68 | 82.82 | 2.21 | 11.84 | 1.00 |
| 9.48 | 84.65 | 2.13 | 12.11 | 0.93 |

**Table S2. The form factors and their fitting parameters for the 100% basic DVB-PS-PDMAEMA series.** The Guinier region was fit to Q\*I(Q) < 1.3. When fitting the data with the PCS model, we used SLD=9.4\*10-6 Å-2 for water. The scattering length density (SLD) was determined to be <SLD RC>=9.94; <SLD RS1>=8.48; <SLD RS2>=10.32.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Form Factor** | **Guinier** | **Star Polymer** | **Polydisperse Core Shell** | **Fit** |
| **pH** | **Rg (Å)** | **α** | **ξ (Å)** | **RC (Å)** | **RS1 (Å)** | **RS2 (Å)** | **Rg (Å)** | χ2**/Npts** |
| 3.18 | 114.51 | 2.10 | 13.20 |  |  |  |  | 0.65 |
| 3.41 | 107.55 | 2.01 | 12.37 |  |  |  |  | 0.60 |
| 4.81 | 105.91 | 2.03 | 12.83 |  |  |  |  | 0.97 |
| 5.72 | 100.12 | 2.00 | 15.84 |  |  |  |  | 0.56 |
| 6.15 | 88.78 | 1.83 | 10.34 |  |  |  |  | 0.78 |
| 7.48 | 85.49 |  |  | 52.30 | 30.10 | 28.90 | 83.31 | 0.80 |
| 7.98 | 92.47 |  |  | 56.15 | 30.50 | 28.70 | 91.93 | 1.01 |
| 8.48 | 91.25 |  |  | 53.00 | 34.40 | 36.65 | 89.47 | 0.98 |
| 8.93 | 84.16 |  |  | 50.06 | 30.49 | 32.01 | 80.66 | 0.88 |
| 9.51 | 88.57 |  |  | 49.15 | 30.72 | 36.52 | 84.11 | 0.70 |

**Table S3. The form factors and their fitting parameters for the 50% basic DVB-PS-PDMAEMA50%/PEGMA50% series.** The Guinier region was fit to Q\*I(Q) < 1.3. When fitting the data with the PCS model, we used SLD=9.4\*10-6 Å-2 for water. The scattering length density (SLD) was determined to be <SLD RC>=9.96; <SLD RS1>=8.55; <SLD RS2>=10.25.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Form Factor** | **Guinier** | **Star Polymer** | **Polydisperse Core Shell** | **Fit** |
| **pH** | **Rg (Å)** | **α** | **ξ (Å)** | **RC (Å)** | **RS1 (Å)** | **RS2 (Å)** | **Rg (Å)** | χ2**/Npts** |
| 2.80 | 100.22 | 1.91 | 14.69 |  |  |  |  | 1.00 |
| 3.51 | 99.42 | 1.89 | 15.45 |  |  |  |  | 0.99 |
| 4.54 | 98.11 | 1.83 | 15.33 |  |  |  |  | 0.98 |
| 4.75 | 85.65 |  |  | 55.79 | 33.81 | 46.48 | 80.19 | 0.99 |
| 6.18 | 80.99 |  |  | 59.85 | 29.31 | 45.14 | 76.51 | 0.45 |
| 8.31 | 81.17 |  |  | 46.43 | 39.93 | 46.12 | 76.12 | 0.79 |
| 8.41 | 79.45 |  |  | 51.13 | 22.23 | 41.62 | 73.76 | 0.82 |
| 9.85 | 79.60 |  |  | 56.19 | 19.94 | 30.41 | 74.23 | 0.42 |

**Table S4. The form factors and their fitting parameters for the 50% acidic DVB-PS-PMAA50%/PEGMA50% series.** The Guinier region was fit to Q\*I(Q) < 1.3. When fitting the data with the PCS model, we used SLD=9.4\*10-6 Å-2 for water. The scattering length density (SLD) was determined to be <SLD RC>=9.90; <SLD RS1>=8.43; <SLD RS2>=10.15.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Form Factor** | **Guinier** | **Star Polymer** | **Polydisperse Core Shell** | **Fit** |
| **pH** | **Rg (Å)** | **α** | **ξ (Å)** | **RC (Å)** | **RS1 (Å)** | **RS2 (Å)** | **Rg (Å)** | χ2**/Npts** |
| 5.11 | 74.33 |  |  | 38.71 | 46.45 | 38.52 | 71.17 | 0.43 |
| 6.38 | 77.12 |  |  | 41.69 | 39.20 | 41.88 | 72.56 | 0.97 |
| 6.48 | 76.54 |  |  | 37.26 | 47.49 | 42.52 | 75.55 | 0.35 |
| 7.03 | 76.00 |  |  | 38.08 | 47.49 | 40.79 | 74.60 | 0.56 |
| 7.04 | 77.10 |  |  | 43.30 | 38.28 | 43.89 | 73.12 | 0.44 |
| 8.03 | 88.10 |  |  | 36.62 | 44.41 | 42.72 | 82.01 | 0.88 |
| 8.66 | 101.04 | 2.22 | 13.01 | 41.57 | 41.48 | 56.83 | 139.88 | 1.14 |
| 9.85 | 121.35 | 2.24 | 11.13 |  |  |  |  | 0.86 |

**Table S5. The form factors and their fitting parameters for the 100% acidic DVB-PS-PMAA series.** The Guinier region was fit to Q\*I(Q) < 1.3.

|  |  |  |  |
| --- | --- | --- | --- |
| **Form Factor** | **Guinier** | **Excluded volume polymer** |  |
| **pH** | **Rg (Å)** | **Rg (Å)** | ***ν*** | χ2**/Npts** |
| 2.91 | 136.10 | 127.75 | 0.588 | 0.98 |
| 3.47 | 112.14 | 102.42 | 0.588 | 0.83 |
| 3.91 | 109.45 | 95.23 | 0.588 | 0.75 |
| 4.48 | 122.06 | 132.00 | 0.588 | 0.99 |
| 5.01 | 124.42 | 123.05 | 0.588 | 0.94 |
| 5.47 | 103.66 | 102.45 | 0.588 | 0.91 |
| 5.95 | 118.76 | 97.23 | 0.588 | 0.95 |
| 6.43 | 116.04 | 102.13 | 0.588 | 0.89 |
| 7.13 | 124.64 | 101.13 | 0.654 | 0.99 |
| 7.46 | 105.46 | 100.21 | 0.588 | 0.95 |
| 7.95 | 99.12 | 103.42 | 0.588 | 0.92 |
| 8.61 | 112.13 | 107.21 | 0.588 | 0.84 |
| 9.07 | 119.81 | 112.34 | 0.588 | 0.99 |
| 9.55 | 121.04 | 125.19 | 0.588 | 0.65 |
| 9.99 | 135.86 | 135.61 | 0.588 | 0.74 |
| 10.93 | 125.04 | 119.91 | 0.588 | 0.84 |
| 12.30 | 122.74 | 111.68 | 0.588 | 0.88 |