

Electronic Supplementary Information

Cationic Polymer Brush-Modified Cellulose Nanocrystals for High-Affinity Virus Binding

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Calculation of CNC surface chain fraction and degree of substitution after α -bromoisobutyryl bromide modification

The dimensions of the pristine CNCs and the ratio of surface chains to the total number of chains in the crystal (approximately 32%) were previously determined.¹

To calculate the degree of substitution (DS) on the initiator-modified CNC-iBBr, we approximated the amount of surface chains to be 1/3 of all cellulose chains in the CNCs. Elemental analysis gave a bromine content of 4.14 (mass-%). The degree of substitution of CNC-iBBr was calculated according to a previously published method.² The DS for the whole CNC-iBBr can be calculated from the following equation, where DS = degree of substitution and Br = bromine content (0.0414).

$$Br = \frac{79.90 \cdot DS}{12.01 \cdot (6 + DS \cdot 3) + 1.008 \cdot (10 + DS \cdot 5) + 16.00 \cdot (5 + DS) + 79.90 \cdot DS}$$

$$\rightarrow 79.90 \cdot DS = 162.14 \cdot Br + 136.97 \cdot DS \cdot Br$$

$$\rightarrow DS \approx 0.09$$

Thus the degree of substitution for the whole modified CNC-iBBr is approximately 0.09.

Considering that the modification only happens on the surface chains, that consist about 1/3 of all chains, we can assume that the DS on the surface is approximately 0.27.

Molar mass of the CNC-iBBr is thus approximately $0.91 \times 162.15 \text{ g/mol} + 0.09 \times 311.14 \text{ g/mol} = 175.56 \text{ g/mol}$.

¹H NMR spectra of SI-ATRP reaction mixtures at 0 min and 120 min

Monomer conversions were determined by ¹H NMR in CDCl₃ for both the 120 and 240 min samples by comparing the monomer vinyl signals (5.49 ppm and 6.04 ppm) to the polymer pendant methyl signal (0.83-0.98 ppm). Other monomer signals are present at 1.87 ppm (-CCH₃), 2.23 ppm (-N(CH₃)₂), 2.55 ppm (-CH₂NMe₂), 4.18 ppm (-OCH₂-) and poly(DMAEMA) signals at 1.75 ppm (backbone -CH₂-), 2.23 ppm (-N(CH₃)₂), 2.55 ppm (-CH₂NMe₂) and 3.98 ppm (-OCH₂-). DMF signals appear at 2.81 ppm, 2.89 ppm and 7.94 ppm.

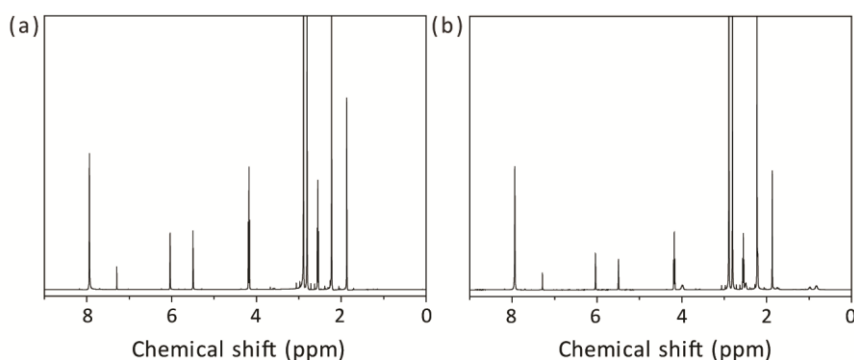


Figure S1. ¹H NMR spectra of the SI-ATRP reaction mixture (a) after 0 minutes and (b) after 120 minutes.

Conversion of the DMAEMA monomer during polymerization based on ^1H NMR

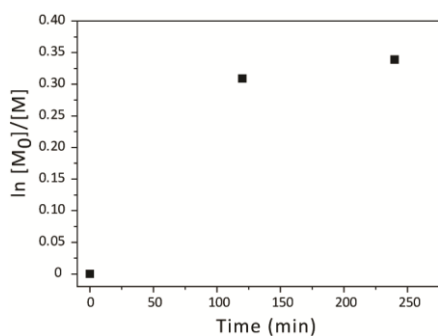


Figure S2. Semilogarithmic plot for monomer conversion versus time. The initial and remaining monomer amounts M_0 and M were determined using ^1H NMR.

Dynamic light scattering of CNC and CNC-*g*-P(QDMAEMA)

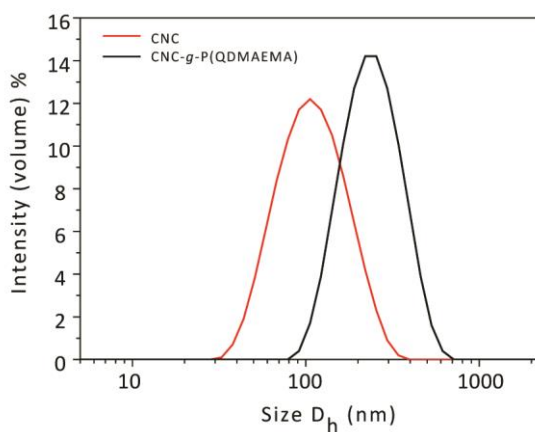


Figure S3. Volume-averaged size distribution profiles for pristine CNCs and CNC-*g*-P(QDMAEMA) in water (0.5 mg/mL).

TEM images of NoV-VLPs and their complexes with CNC-g-P(QDMAEMA) at 0 mM NaCl

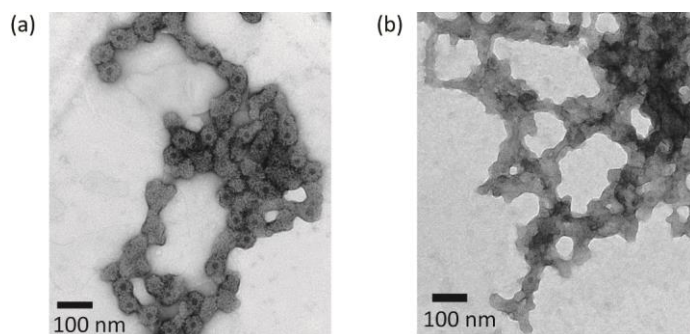


Figure S4. TEM micrographs of (a) NoV-VLP at 0 mM NaCl. (b) Complexes of CNC-g-P(QDMAEMA) and NoV-VLP at 0 mM NaCl.

References

1. H. Rosilo, E. Kontturi, J. Seitsonen, E. Kolehmainen and O. Ikkala, *Biomacromolecules*, 2013, **14**, 1547.
2. C. Vaca-Garcia, M. E. Borredon and A. Gaseto, *Cellulose*, 2001, **8**, 225.