Supporting Information

Characterization of Polymer-Silica Nanocomposite Particles with Core-Shell Morphologies using Monte Carlo Simulations and Small Angle X-ray Scattering

Jennifer A. Balmer, Oleksandr O. Mykhaylyk*, Andreas Schmid, Steven P. Armes*, J. Patrick A. Fairclough and Anthony J. Ryan

Dainton Building, Department of Chemistry,
The University of Sheffield, Sheffield, Brook Hill, S3 7HF, UK

SAXS analysis of silica aqueous solutions

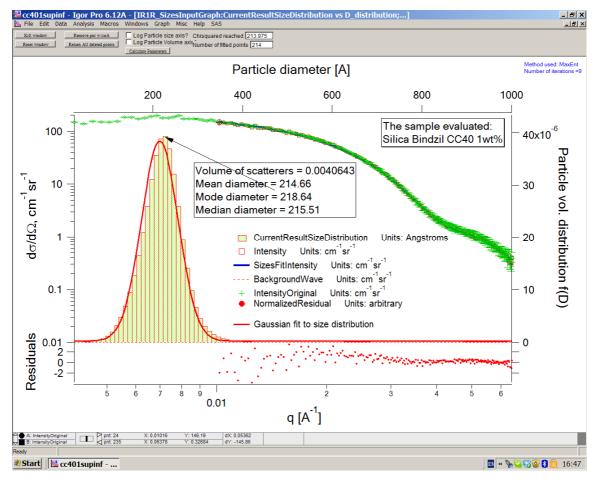


Figure S1. Silica particles size analysis. A screenshot of Irena SAS macros for Igor Pro after analysis of SAXS pattern of 1 wt% aqueous dispersion of Bindzil CC40 silica nanoparticles by the maximum entropy method available for particle size distribution analysis in this software. It is assumed that the silica particles have a spherical morphology. The particle size distribution histogram has Gaussian character (red line).

^{*} Authors to whom correspondence should be addressed: O.Mykhaylyk@sheffield.ac.uk and S.P.Armes@sheffield.ac.uk

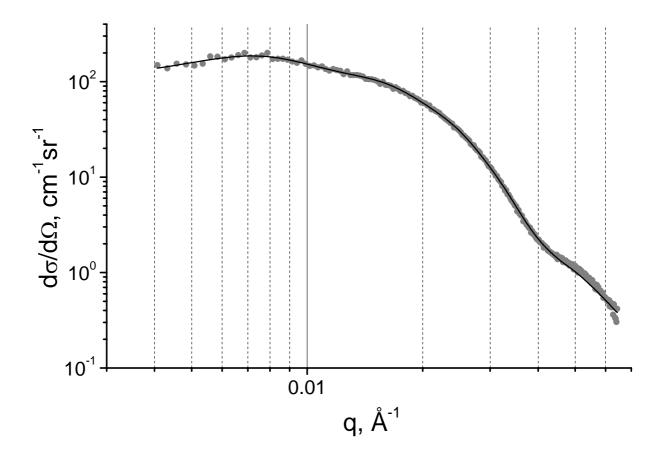


Figure S2. SAXS results obtained for a 1.0 wt% aqueous dispersion of Bindzil CC40 silica nanoparticles: grey circles indicate the experimental scattering profile and the solid line represents the fitting curve. It is assumed in the model that the silica particles are spherical, their size polydispersity has a Gaussian distribution, the interparticle interference of the silica in the solution is described by a hard-sphere Percus-Yevick model, the mass density of the silica is 2.19 g cm⁻³, the mass density of the water is 1.00 g cm⁻³, the scattering length densities for the silica (ξ_{silica}) and water (ξ_{sol}) are 18.56×10^{10} cm⁻² and 9.581×10^{10} cm⁻², respectively. The following structural parameters have been obtained: R_{silica} (mean silica particle radius) = 108 Å; σ_{silica} (standard deviation of the silica particle radius) = 22 Å; c_{silica} (volume fraction of the silica particles) = 0.0041, corresponding to a silica particle concentration in the dispersion of 0.89 wt%; R_{PY} (Percus-Yevick hard-sphere radius of the silica in the aqueous solution) = 375 Å and c_{PY} (Percus-Yevick volume fraction of silica) = 0.095.