Electronic Supplementary Material (ESI) for CrystEngComm

Supporting information

Facile preparation of $CaCO_3$ nanocrystals with unique morphologies controlled by supramolecular complexes

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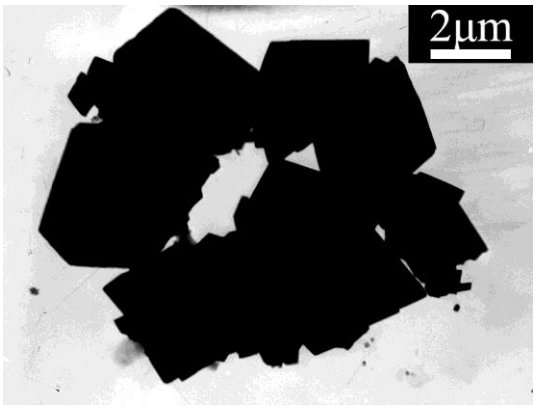


Figure S1. TEM image of $CaCO_3$ nanostructures obtained in the absence of DTAB when the concentration of β-CD was 1.0 mM.

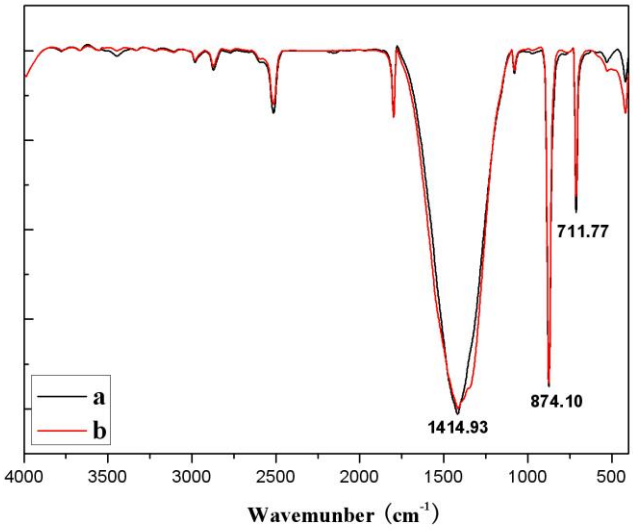


Figure S2. FTIR spectra recorded from the $CaCO_3$ nanocrystals used as the reference (curve a) and the $CaCO_3$ nanostructures shown in Figure 1C (curve b).

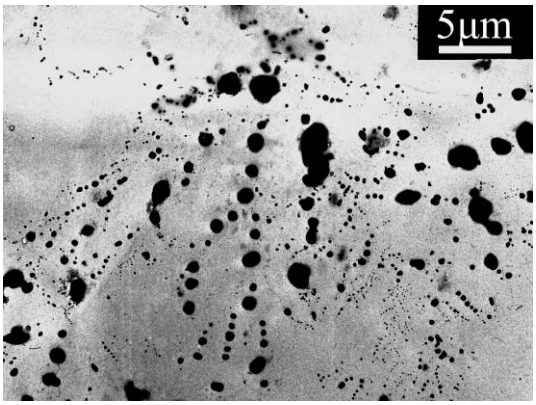


Figure S3. TEM image of $CaCO_3$ nanostructures obtained without initial incubation of the β-CD/DTAB solution. [DTAB] = 1.0 mM; [β-CD] = 1.0 mM.

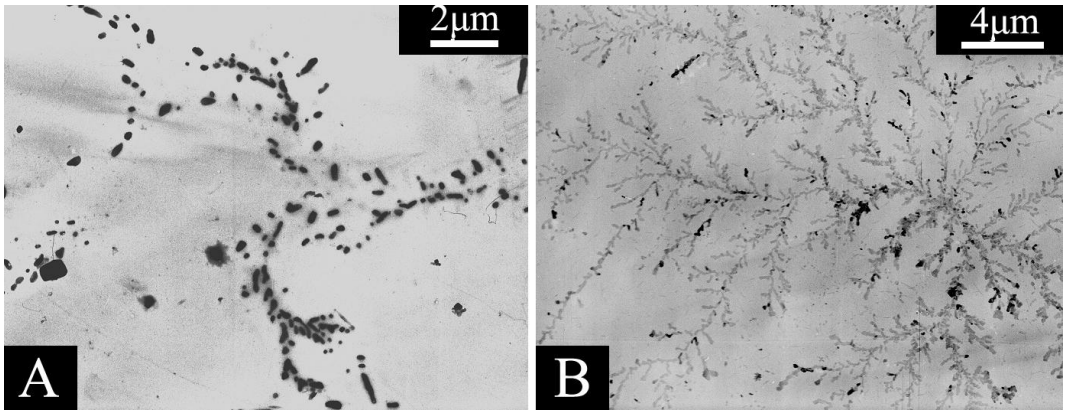


Figure S4. TEM images of $CaCO_3$ products obtained in mixed β-CD/DTAB solutions at various DTAB concentrations when the molar ratio of β-CD-to-DTAB was 1.0. [DTAB]: (A) 0.5 mM; (B) 5.0 mM.

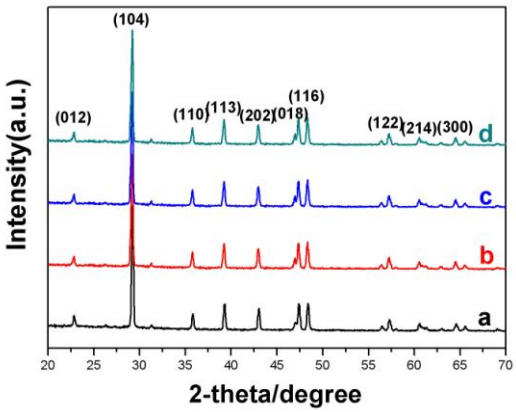
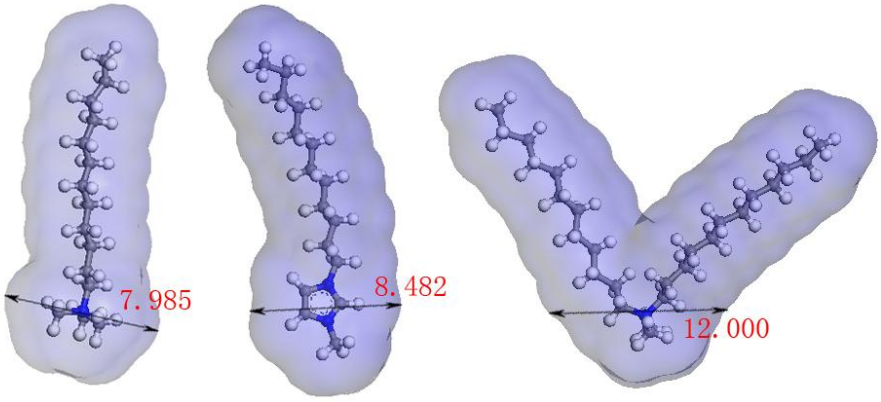


Figure S5. XRD patterns characteristics of the $CaCO_3$ crystals obtained in C_{12}minBr (A), mixed β-CD/C_{12}minBr (B), DDAB (C), and mixed β-CD/DDAB (D) solutions. [C_{12}minBr] = 1.0 mM, [β-CD]/[C_{12}minBr] = 1.0; [DDAB] = 1.0 mM, [β-CD]/[DDAB] = 1.0.



DTAB **C_{12}mimBr** **DDAB**

Figure S6. Optimized conformers of the three surfactants.

In order to further reflect the influence of the steric effects, the Connolly surface [S1] was calculated to show the approximate values of sectional area using a water molecule (as a sphere of radius 1.4 Å) as the probe. From the calculation, the diameters of the hydrophilic head are obtained, which are shown in Fig.S6.

References

[S1] (a) S. M. Yuan, H. Yan, K. Lv, C. B. Liu and S. L. Yuan, *J. Colloid Interface Sci.* 2010, **348**, 159. (b) M. L. Connolly, *Science* 1983, **221**, 709.