

SUPPLEMENTARY MATERIAL TO
**Molecular modelling of zinc sulphide nanoparticles stabilized by
cetyltrimethylammonium bromide**

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J. Serb. Chem. Soc. 79 (12) (2014) 1545–1559

ADDITIONAL FIGURES AND TABLES

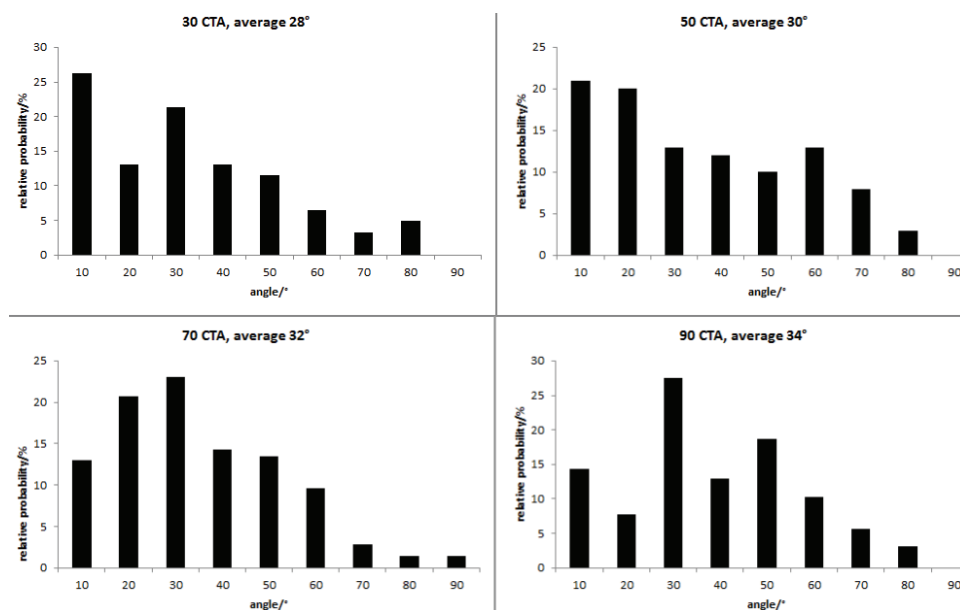


Fig. S-1. Angle distribution of the CTAs in model 1 without water.

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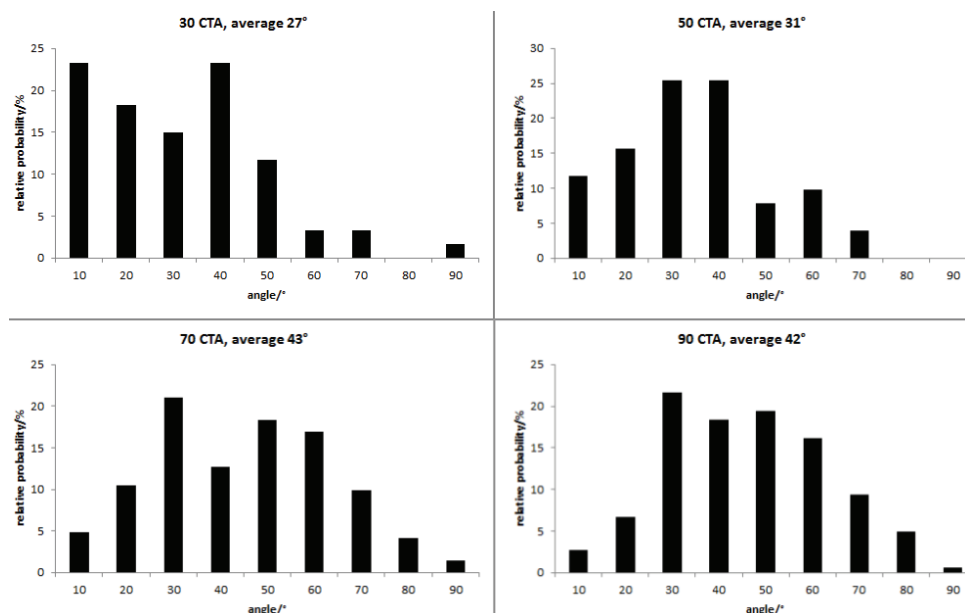


Fig. S-2. Angle distribution of CTAs in model 2 without water.

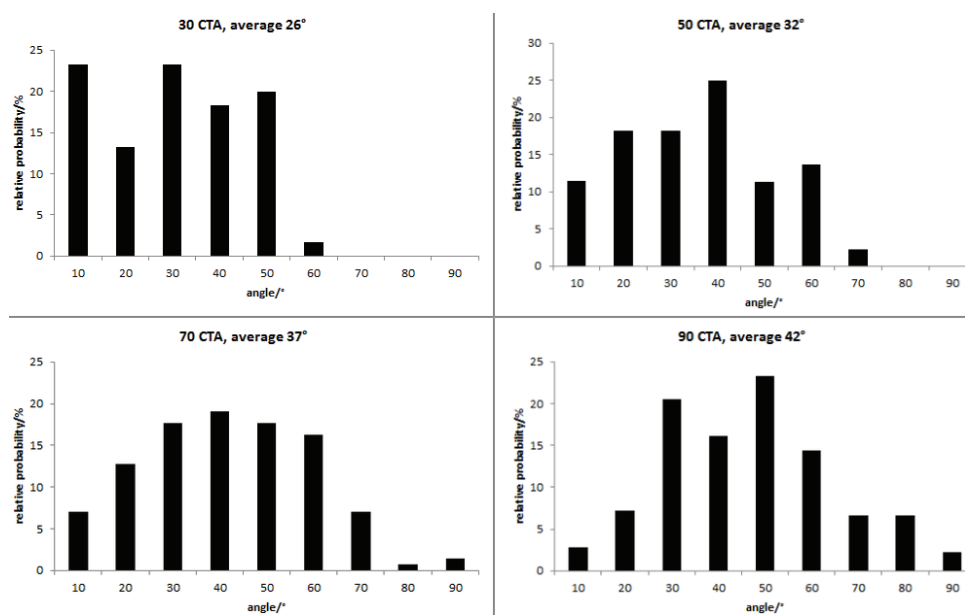


Fig. S-3. Angle distribution of CTAs in model 3 without water.

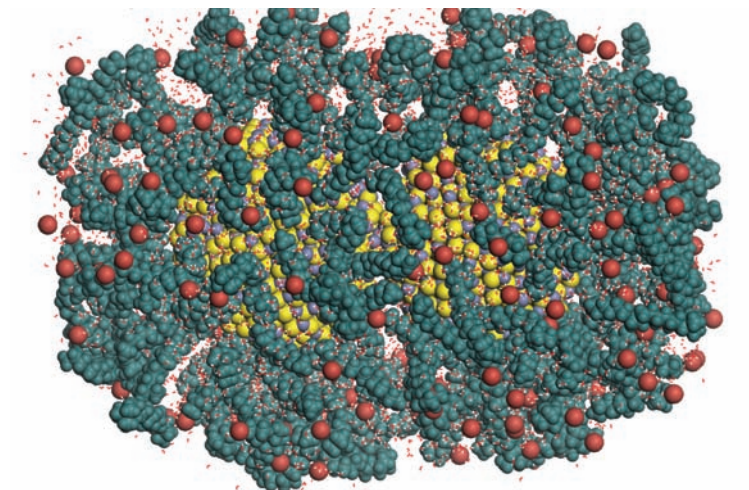


Fig. S-4. A ZnS nanoparticle covered with 90 CTAs, simulated according to Model 1. The green chains represent CTA cations and the brown balls represent bromide anions.

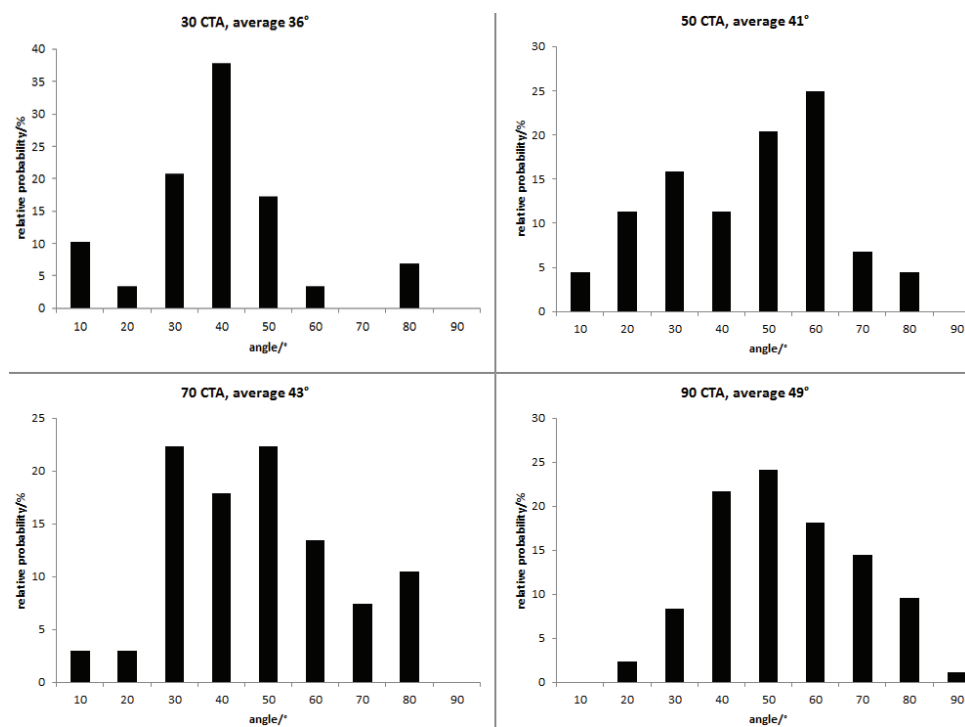


Fig. S-5. Angle distribution of the CTAs in model 2 with water.

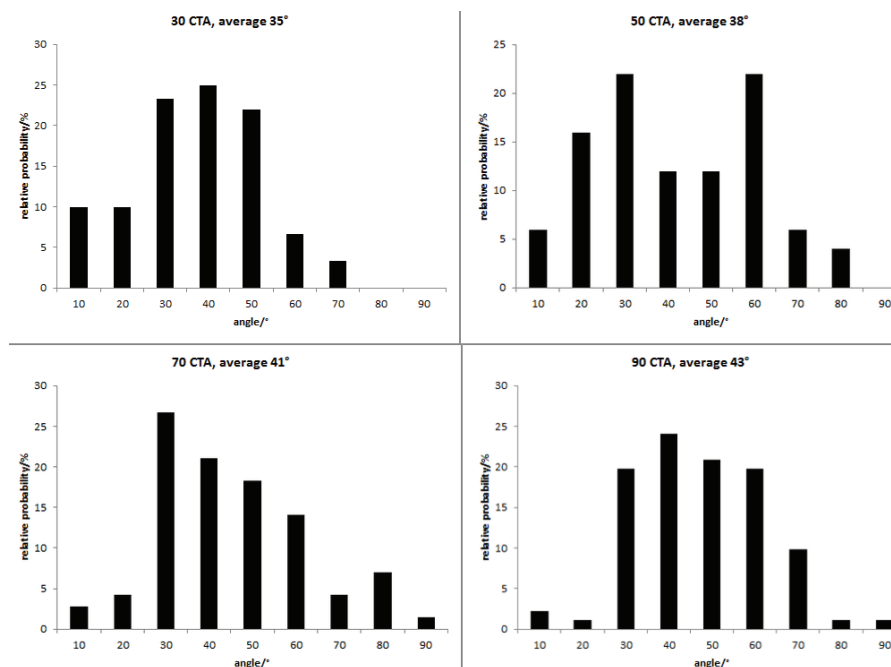


Fig. S-6. Angle distribution of the CTAs in model 3 with water.

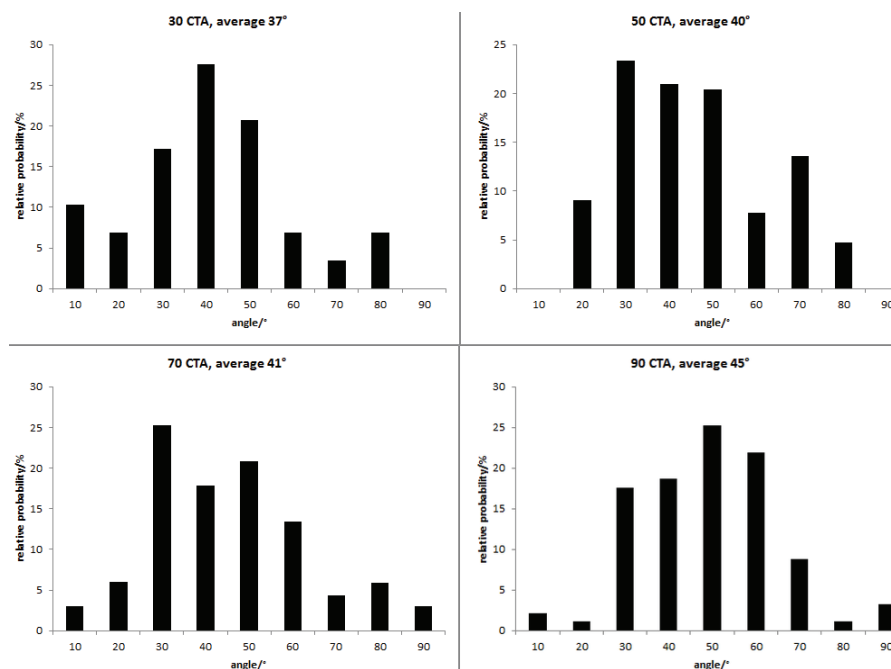


Fig. S-7. Angle distribution of the CTAs in model 4 with water.

TABLE S-1. Nonbonded interactions and their components for the models without water

Model type	CTA amount	Interaction	$E_{\text{total}} / \text{kcal}^* \text{mol}^{-1}$	$E_{\text{vdw}} / \text{kcal mol}^{-1}$	$E_{\text{elst}} / \text{kcal mol}^{-1}$
1	30	Total	-2431	-252	-2179
		CTA-CTA	-99	-140	41
		ZnS-CTA	-2116	-106	-2010
		ZnS-ZnS	-215	-5	-210
2		Total	-2894	-308	-2586
		CTA-CTA	-147	-148	1
		ZnS-CTA	-2747	-159	-2588
3		Total	-2820	-248	-2572
		CTA-CTA	-97	-107	10
		ZnS-CTA	-2723	-141	-2582
4		Total	-2992	-284	-2708
		CTA-CTA	-231	-171	-60
		ZnS-CTA	-2761	-114	-2647
1	50	Total	-2935	-523	-2412
		CTA-CTA	266	-365	631
		ZnS-CTA	-3107	-148	-2959
		ZnS-ZnS	-94	-9	-85
2		Total	-3683	-556	-3127
		CTA-CTA	308	-334	642
		ZnS-CTA	-3991	-222	-3769
3		Total	-3479	-426	-3053
		CTA-CTA	-81	-257	176
		ZnS-CTA	-3398	-169	-3229
4		Total	-3930	-473	-3457
		CTA-CTA	-177	-247	70
		ZnS-CTA	-3753	-225	-3528
1	70	Total	-2597	-909	-1688
		CTA-CTA	1336	-753	2089
		ZnS-CTA	-3802	-146	-3656
		ZnS-ZnS	-131	-9	-122
2		Total	-2601	-54	-2547
		CTA-CTA	1205	-740	1945
		ZnS-CTA	-3806	686	-4492
3		Total	-3803	-790	-3013
		CTA-CTA	535	-599	1134
		ZnS-CTA	-4338	-190	-4148
4		total	-4026	-902	-3124
		CTA-CTA	393	-705	1098
		ZnS-CTA	-4419	-197	-4222
1	90	total	-2452	-1401	-1051
		CTA-CTA	2168	-1196	3364
		ZnS-CTA	-4242	-198	-4044
		ZnS-ZnS	-378	-7	-371

* 1 kcal = 4.184 kJ

TABLE S-1. Continued

Model type	CTA amount	Interaction	$E_{\text{total}} / \text{kcal mol}^{-1}$	$E_{\text{vdw}} / \text{kcal mol}^{-1}$	$E_{\text{elst}} / \text{kcal mol}^{-1}$
2		total	-3562	-1311	-2251
		CTA-CTA	1719	-1074	2793
		ZnS-CTA	-5281	-237	-5044
3		total	-3716	-1216	-2500
		CTA-CTA	1189	-967	2156
		ZnS-CTA	-4905	-248	-4657
4		total	-4022	-1249	-2773
		CTA-CTA	1116	-1011	2127
		ZnS-CTA	-5138	-239	-4899

TABLE S-II. Nonbonded interactions obtained by the simulations for the models with water

Number of CTA	$E_{(\text{ZnS-CTA})+\text{Br}+\text{H}_2\text{O}} / \text{kcal mol}^{-1}$	$E_{\text{H}_2\text{O}} / \text{kcal mol}^{-1}$	$E_{\text{ZnS}+\text{H}_2\text{O}} / \text{kcal mol}^{-1}$
Model 1			
30	-488140	-439046	-19900
50	-503913	-433381	-20729
70	-513910	-427110	-19813
90	-529874	-422786	-21034
Model 2			
30	-483663	-438661	-19649
50	-470433	-406874	-18787
70	-487375	-409768	-17120
90	-521702	-420507	-19629
Model 3			
30	-454654	-407826	-18770
50	-468993	-403851	-19358
70	-479255	-396095	-20699
90	-490624	-393556	-19594
Model 4			
30	-459347	-412522	-20010
50	-444415	-383126	-19019
70	-467141	-388087	-18024
90	-500200	-397597	-18827