INVESTIGATING THE SPONTANEOUS FORMATION OF SDS MICELLE IN AQUEOUS SOLUTION USING A COARSE-GRAINED FORCE FIELD

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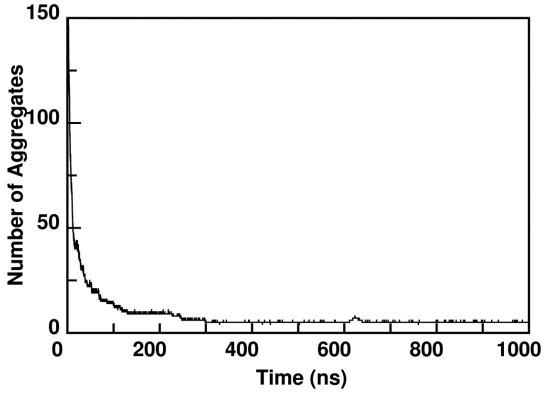

Figure 1S. *Total number of SDS aggregates during the simulation (including monomers and premicellar aggregates)*

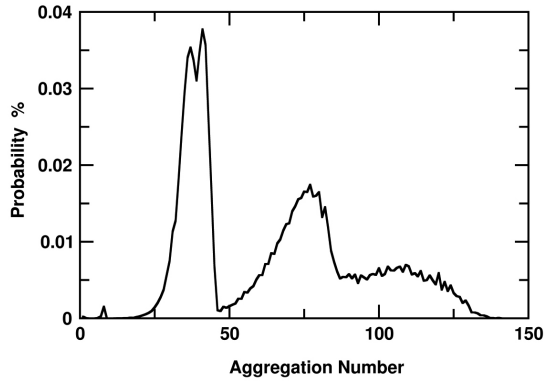

Figure 2S. *Cluster size probability distribution*

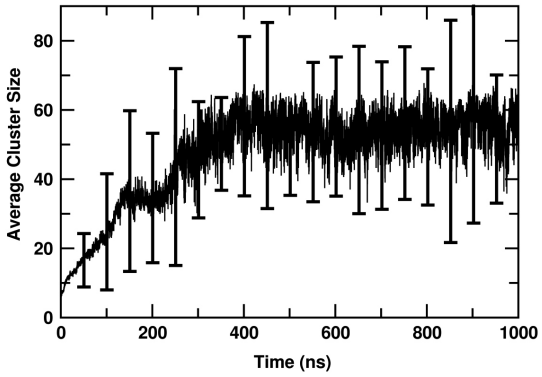

Figure 3S. *Average aggregation number of the micellar aggregates*

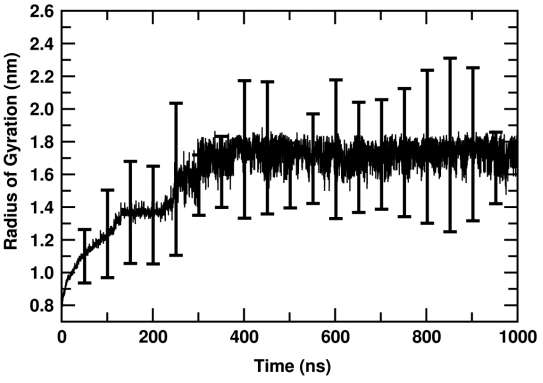

Figure 4S. *Average radius of gyration of the micellar aggregates*

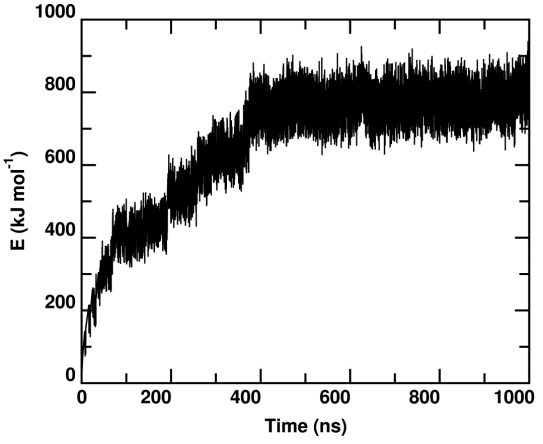

Figure 5S. *Coulomb energy between Na^+ cation from 0.0 up to 1000 ns simulation*

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Table 1S. Micellar parameters: model, SDS molar concentration [SDS], average aggregation number < N > and Radius of SDS micelle < R >

Ref. Year	Method	Model	[SDS] (mM)	< N >	< R > /nm
[43] 1981	SANS	Polydisperse spheres	40		2.17
[45] 1986	SANS	Polydisperse spheres	65	90	2.51
[46] 1999	SANS	Polydisperse spheres	-	48	2.00
[48] 2002	SAXS	Ellipsoid	40	-	2.18
[44] 2005	SANS	Ellipsoid biaxial	50	75	2.23
[42] 2007	SANS SAXS	Ellipsoid triaxial	300	91	2.20
[47] 2009	SANS SAXS	Ellipsoid triaxial core/shell	50	67	2.12
[47] 2009	SANS SAXS	Ellipsoid oblate homogeneous	50	77	2.12
[36] 1995	A.A MD	Spheres	700	60	2.21
[34] 2002	A.A MD	Spheres	400	60	2.20
[26] 2005	AA/CG MD	Spheres	1100	60	2.00 ± 0.01
[37] 2009	CG MD	Spheres	100	60	2.03 ± 0.03
This work	CG MD	Spheres	55	41 68 and 95	2.23 ± 0.08