# Coarse-graining for the Analysis of Soft Matter Scattering

submitted by

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for the degree of Doctor of Philosophy

of the

#### UNIVERSITY OF BATH

Department of Chemistry

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"Atticus told me to delete the adjectives and I'd have the facts."

Scout Finch – To Kill a Mockingbird

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### **Abstract**

Department of Chemistry

Doctor of Philosophy

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### List of Abbreviations

MD molecular dynamics

C<sub>10</sub>TAB decyltrimethylammonium bromide dipalmitoylphosphatidylcholine

**SAS** small angle scattering

**GISAS** grazing-incidence small angle scattering

**SAXS** small angle X-ray scattering

**XRR** X-ray reflectivity

**GISAXS** grazing-incidence small angle X-ray scattering

**SANS** small angle neutron scattering

**NR** neutron reflectivity

GISANS grazing-incidence small angle neutron scattering

**DLS** Diamond Light Source

**ESRF** European Synchrotron Radiation Facility

Linac linear accelerator
BM bending magnet
rf radio-frequency cavity

**ID** insertion device

ILL Institut Laue-LangevinESS European Spallation Source

EPSR emperical potential structure refinement DWBA distorted wave Born approximation

PCFF poly consistent force field PBC periodic boundary condition

**OPLS** optimized potentials for liquid simulations

**NVE** constant number of particles, volume, and energy

NPT constant number of particles, pressure, and temperature NVT constant number of particles, volume, and temperature

**WPEP** whole particle effective potential decyltrimethylammonium nitrate

## **Physical Constants**

 $\pi = 3.14159...$   $c = 2.998 \times 10^8 \,\mathrm{m \, s^{-1}}$   $h = 6.626 \times 10^{-34} \,\mathrm{J \, s}$ Speed of light Planck's constant

Golden ratio  $\Phi = 1.61803\dots$ 

Boltzmann's constant  $k_B = 1.380\,648 \times 10^{-23}\,\mathrm{J\,K^{-1}}$ 

# List of Symbols

$a_0$	optimum head-group area	$\mathrm{m}^2$
b	scattering length	m
b	bond length	m
$b_0$	equilibrium bond length	m
$c_{\alpha/\beta}$	atom concentrations	$\mathrm{m}^{-3}$
$d_n$	thickness of layer $n$	m
f	force	${\rm kgms^{-2}}$
$f_s$	scale factor	
$g_{lphaeta}$	partial pair distribution function	
g(X)	probability density function	
i	atom type	
$k_n$	wavevector for layer $n$	
$k_N$	dissociation constant from aggregate of $N$	$s^{-1}$
$l_0$	chain length	m
m	mass	kg
n	number of scattering vectors	
$n_i$	refractive index	
$q_i$	charge of atom $i$	$k_e$
p	surfactant packing parameter	
$r_c$	cut-off distance	m
$r_{ij}$	atomic distance	Å
$r_{n,n+1}$	Fresnel equation coefficient	0
$r_{12}$	distance between surfactant centres-of-mass	Å
s	surfactant number	
t	timestep	S
$t_F$	time-of-flight	S
u	potential energy	$kJ  mol^{-1}$
v	velocity	$\mathrm{m}\mathrm{s}^{-1}$
A	illuminated surface	$m^2$
$A_{1,2,3}$	dihedral angle parameters	$kcal  mol^{-1}$
B	resultant matrix	
C	total solute concentration	$ m moldm^{-3}$
$C_s$	tail carbon atom in surfactant s	9
D	number density of particles	$\mathrm{m}^{-3}$
$E_k$	kinetic energy	J
$E_{\text{new}}$	new energy	kJ
$E_{\text{tot}}$	total energy	kJ
$F(\mathbf{Q})$	diffuse scattering factors	
G(r)	radial distribution function	_1
$I^{(Q)}$	scattering intensity	$\mathrm{cm}^{-1}$
K	equilibrium constant	
$K_b$	bond force constant	$kcal mol^{-1} Å^{-}$
$K_{\theta}$	angle force constant	$kcal  mol^{-1}$

_		
$L_F$	distance of neutron flight	m
M	layer matrix	
N	aggregation number	molecule
$N_{at}$	number of atoms	
$N_{ m cycles}$	number of cycles	
$N_{\rm particles}$	number of particles	
$N_P$	number of undulator magnets	
$N_s$	head nitrogen atom in surfactant s	
P	probability	
P(Q)	particle form factor	
Q	scattering vector magnitude	$\mathrm{m}^{-1}$
R	radius	m
$R_g$	radius of gyration	m
R(Q)	reflectivity	
Res(Q)	resolution function	
S	nuclear spin quantum number	
$S_a$	surface area	$m^2$
$S_a$ $S(Q)$	system structure factor	111
T	temperature	K
_	<del>-</del>	K
$T_{\rm inst}$	instantaneous temperature Fresnal transmission factor	Λ
$T_{i,f}$		3
V	volume	$\frac{\mathrm{m}^3}{\mathrm{s}}$
$V_c$	chain volume	$m^3$
$V_p$	particle volume	meter <sup>3</sup>
$X_N$	concentration of molecules in aggregate of $N$	$mol dm^{-3}$
$\mathbf{k}_i$	incident wavevector	$\mathrm{m}^{-1}$
$\mathbf{k}_f$	final wavevector	$\mathrm{m}^{-1}$
$\mathbf{r}$	atomic position	_
$\mathbf{Q}$	scattering vector	$\mathrm{m}^{-1}$
β	phase factor	
$\beta_c$	fraction of $c$	
$\delta_{lphaeta}$	Kronecker $\delta$ -function	
*	L-J well depth	$kcal  mol^{-1}$
$rac{\epsilon_{ij}}{ heta}$	polar angle	rad
$\theta$		deg
	angle	_
$\theta_{1/2}$	surfactant- $r_{12}$ angle	deg
$\theta_c$	critical angle	rad
$\theta_e$	electron-photon angle	rad
$\theta_0$	equilibrium angle	deg
$\lambda$	wavelength	m
$\lambda_P$	magnetic period length	m
$\mu$	atomic mass	amu
$\mu_N$	mean chemical potential of aggregate of $N$	J molecule <sup>−1</sup>
$\mu_N^\circ$	mean interaction energy of aggregate of $N$	$J  \text{molecule}^{-1}$
$ u_{\mathrm{samp}}$	sampling frequency	
$\rho$	scattering length density	$\mathrm{m}^{-2}$
$ ho_0$	atomic density	$\mathrm{m}^{-3}$
$\sigma$	interfacial roughness	m
$\sigma_i$	statistical uncertainty in $I^{\exp}(Q)$	${ m cm}^{-1}$
$\sigma_{ij}$	distance of L-J minima	Å
•		

$\sigma_{coh}$	coherent scattering cross section		$1^2$
$\sigma_{ m incoh}$	incoherent scattering cross section	n	$1^2$
$\phi$	azimuthal angle	ra	ad
$\phi$	dihedral angle	ra	ad
$\chi^2$	chi-squared		
$\omega$	neutron frequency	S	-1
$\omega_i$	incident frequency	Н	Iz
$\omega_f$	final frequency	Н	$\mathrm{Iz}$
$\mathrm{d}\sigma/\mathrm{d}\omega$	differential cross-section	m	$1^2$
$\Lambda$	temperature factor		

### **Aims**

#### 0.1 Main Section 1

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#### 0.1.1 Subsection 1

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#### 0.1.2 Subsection 2

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#### 0.2 Main Section 2

### 1 Introduction

#### 1.1 Main Section 1

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### 2 Simulation Methodology

#### 2.1 Main Section 1

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#### 2.2 Main Section 2

# 3 Reflectivity from Lipid Monolayers

#### 3.1 Main Section 1

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#### 3.1.2 Subsection 2

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#### 3.2 Main Section 2

# 4 Small Angle Scattering from Surfactant Micelles

#### 4.1 Main Section 1

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#### 4.2 Main Section 2

# 5 Grazing Incidence Small Angle Scattering from Mixed Surfactant Monolayers

#### 5.1 Main Section 1

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#### 5.2 Main Section 2

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### 6 Conclusions

#### 6.1 Main Section 1

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#### 6.2 Main Section 2

# A Appendix Title Here

Write your Appendix content here.

# **List of Figures**

## **List of Tables**

# List of Algorithms

# Bibliography

[1] A. Test, Another Test.