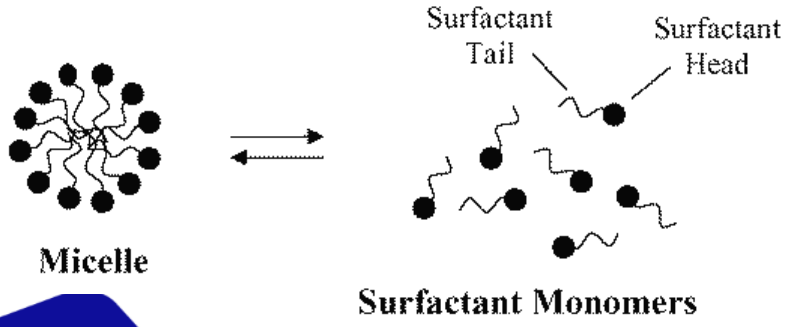
MODELLING FOR INDUSTRIAL APPLICATIONS

COMPUTATIONAL CHEMISTRY FOR SURFACTANT SCIENCE



Dr Massimo Noro
Unilever R&D Port Sunlight

Massimo.Noro@Unilever.com

UNILEVER AT A GLANCE

2bn
consumers worldwide use a Unilever product on any day

53%
of sales in emerging markets

Products sold in more than 180 countries

More than 50 years experience in Brazil, China, India and Indonesia

THE TEAM:

Patrick Warren, Ian Stott

Bill Swope, Michael Johnston, Kirk Jordan

Rick Anderson, David Bray, Annalaura Del Regno

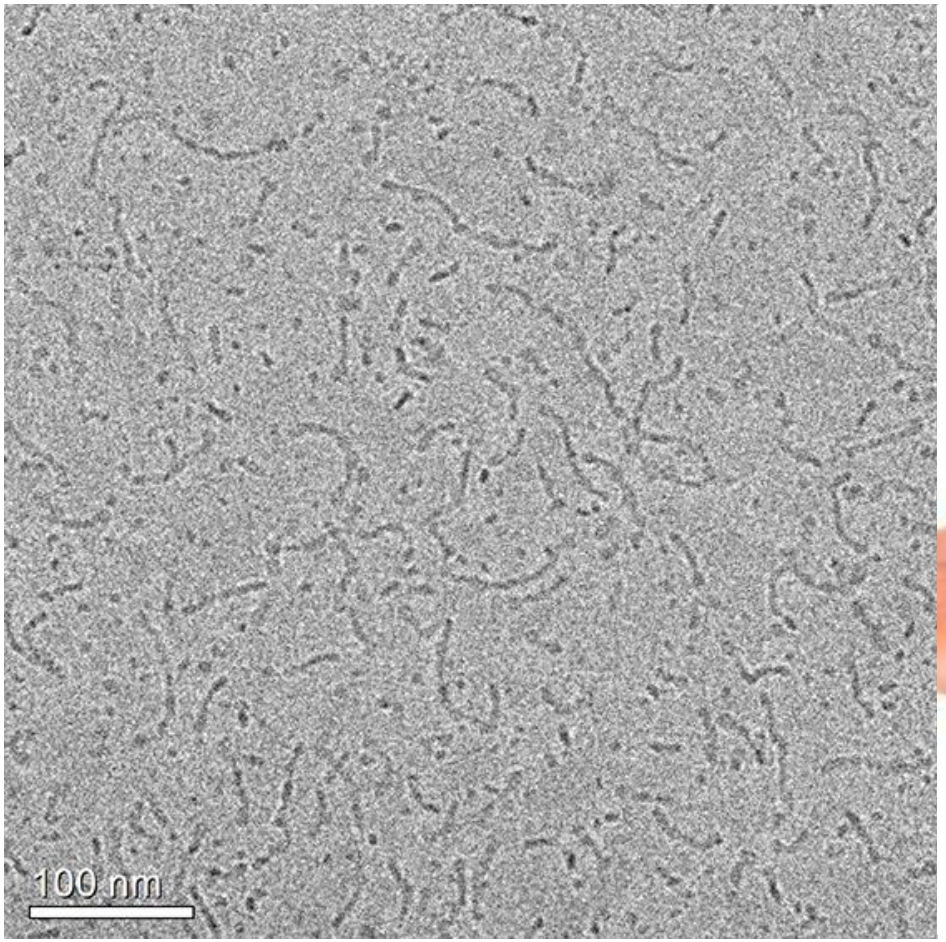
OUTLINE

1. Industrial challenges in surfactant science
2. Mesoscale computational approach
3. Applications:
    - phase behaviour
    - micellar properties
4. Deploying to end-users

SURFACTANTS FOR WASHING YOUR HAIR

FOR FULLER, THICKER LOOKING HAIR**

HOW TO BUILD AND MAINTAIN VISCOSITY ?

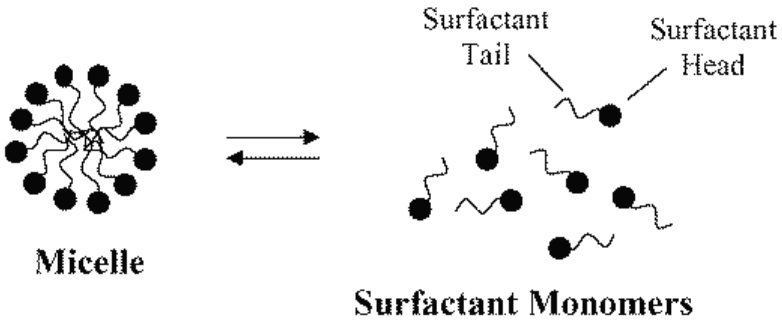


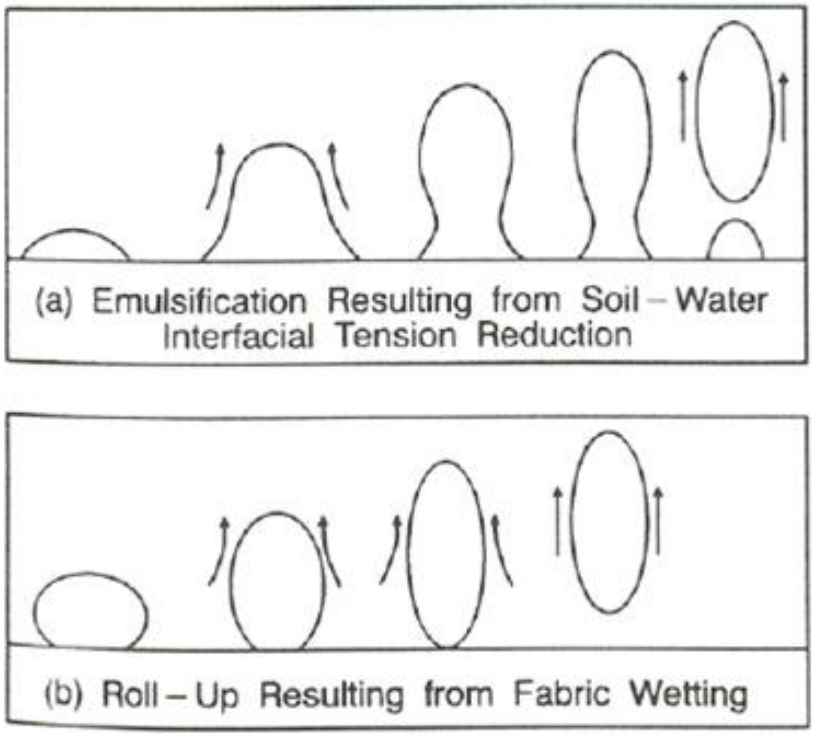
Unpublished – collaboration with University of Sofia

SURFACTANTS FOR DOING THE LAUNDRY

HOW TO PREDICT:

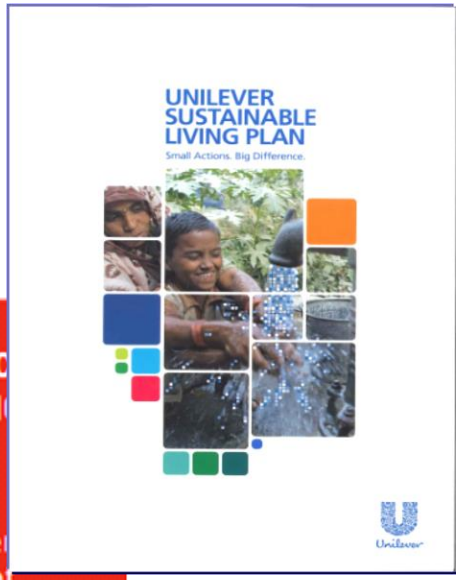
MICELLE FORMATION CLEANING EFFICIENCY?





From Miller & Raney, Coll. Surf A 74, 169-215 (1993)
"Solubilisation-emulsification mechanisms of detergency"

VIEW TO THE FUTURE: "NATURAL" SURFACTANTS?



IMPROVING HEALTH AND WELL-BEING

By 2020 we will help more than a billion people take action to improve their health and well-being.

REDUCING ENVIRONMENTAL IMPACT

By 2020 our goal is to halve the environmental footprint of the making and use of our products as we grow our business.*

ENHANC LIVELIH

By 2020 we will e the livelihoods o hundreds of thousands of people as we grow our business.

HEALTH & HYGIENE >>

IMPROVING NUTRITION >>

GREENHOUSE GASES >>

WATER >>

WASTE >>

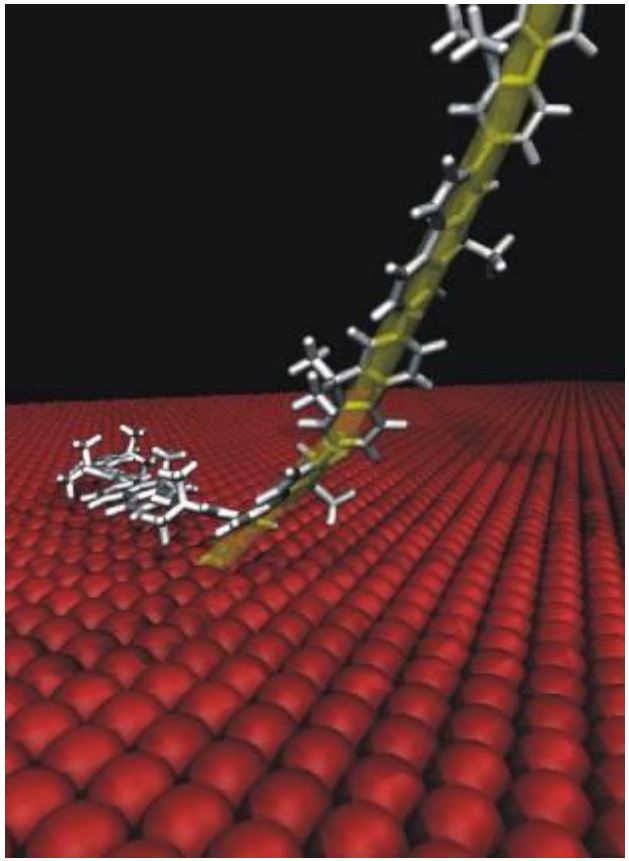
SUSTAINABLE SOURCING >>

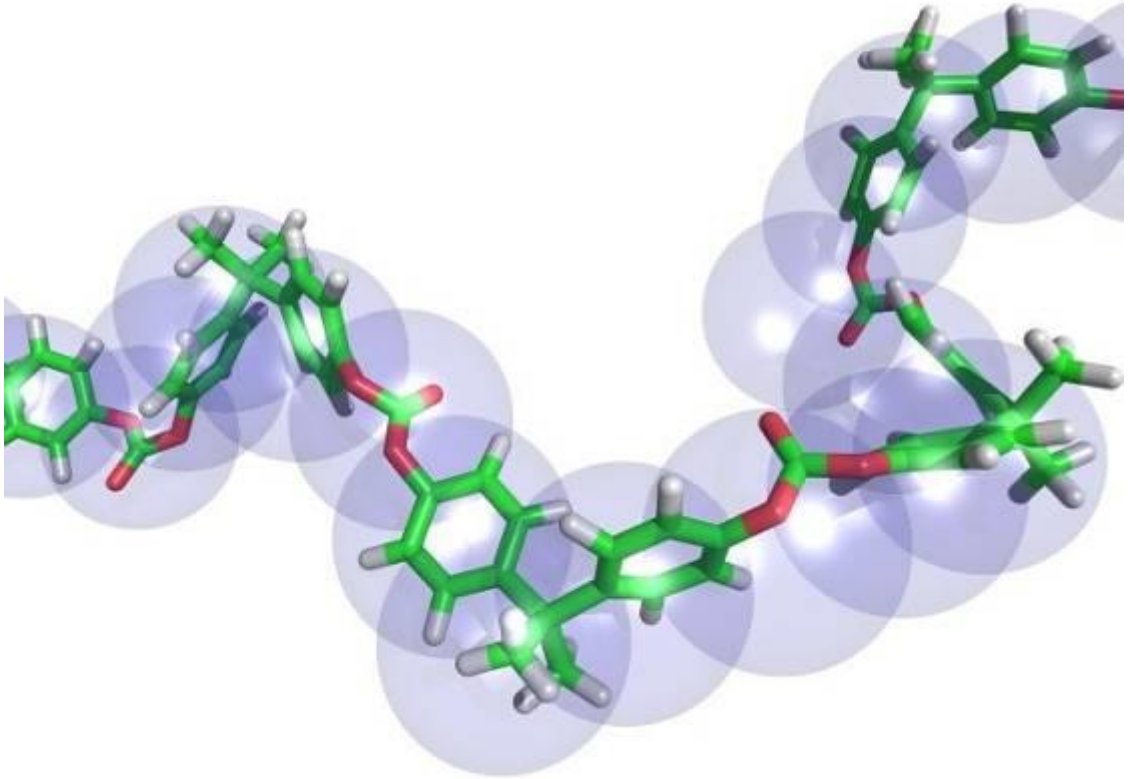
BETTER LIVELIHOODS >>

http://unilever.com/sustainable-living/index.aspx

MODELLING APPROACHES

Atomistic ⟷ **Mesoscale**





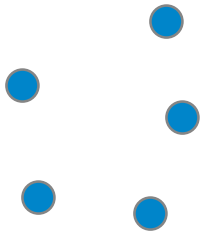
One millionth of a second (10^{-6}s)

Seconds

DISSIPATIVE PARTICLE DYNAMICS

Unilever

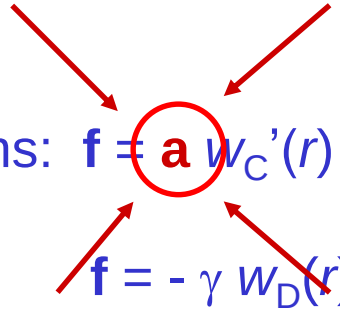
Particles



Positions $\mathbf{r}_i$, velocities $\mathbf{v}_i = d\mathbf{r}_i/dt$

Newton's E.O.M, $m\, d\mathbf{v}_i/dt = \mathbf{f}_i$

Interaction laws

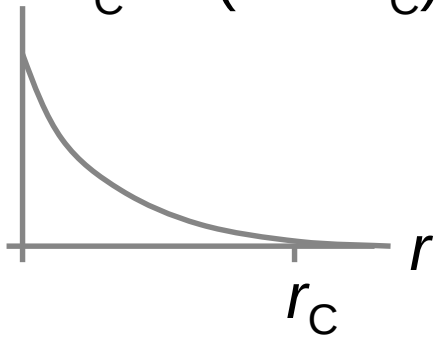


Soft pairwise repulsions: $\mathbf{f} = \mathbf{a}\, w_C'(r)\, \mathbf{e}$

Pairwise drag forces: $\mathbf{f} = -\gamma\, w_D(r)\, (\mathbf{v}.\mathbf{e})\, \mathbf{e}$

Pairwise random forces, determined by FD and kT

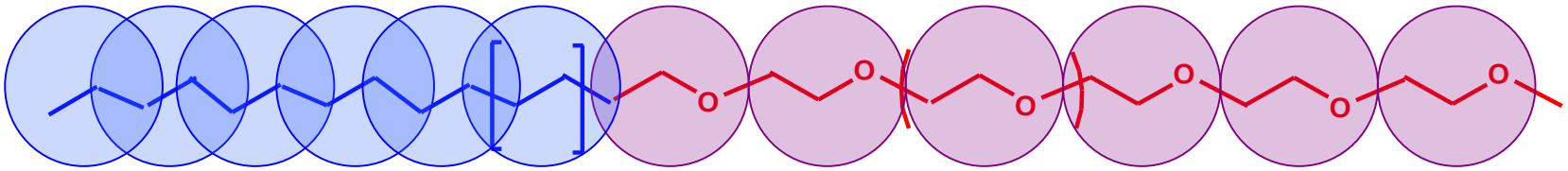
$w_D = w_C = (1 - r/r_C)^2$



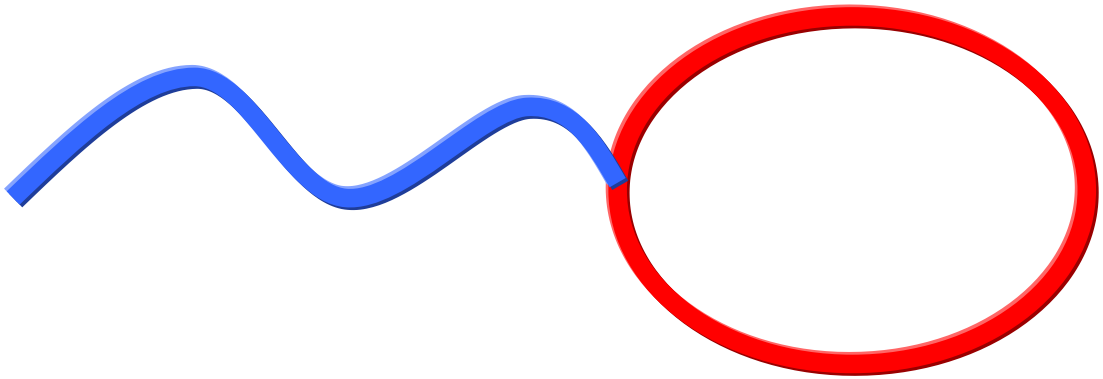
Parameters : $m = r_C = kT = 1$, remaining ρ, γ, a

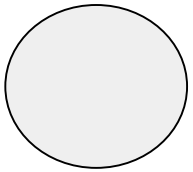
P. Español and P. B. Warren, Europhys. Lett. **30** (1995) 191

A TYPICAL "LAUNDRY" DETERGENT

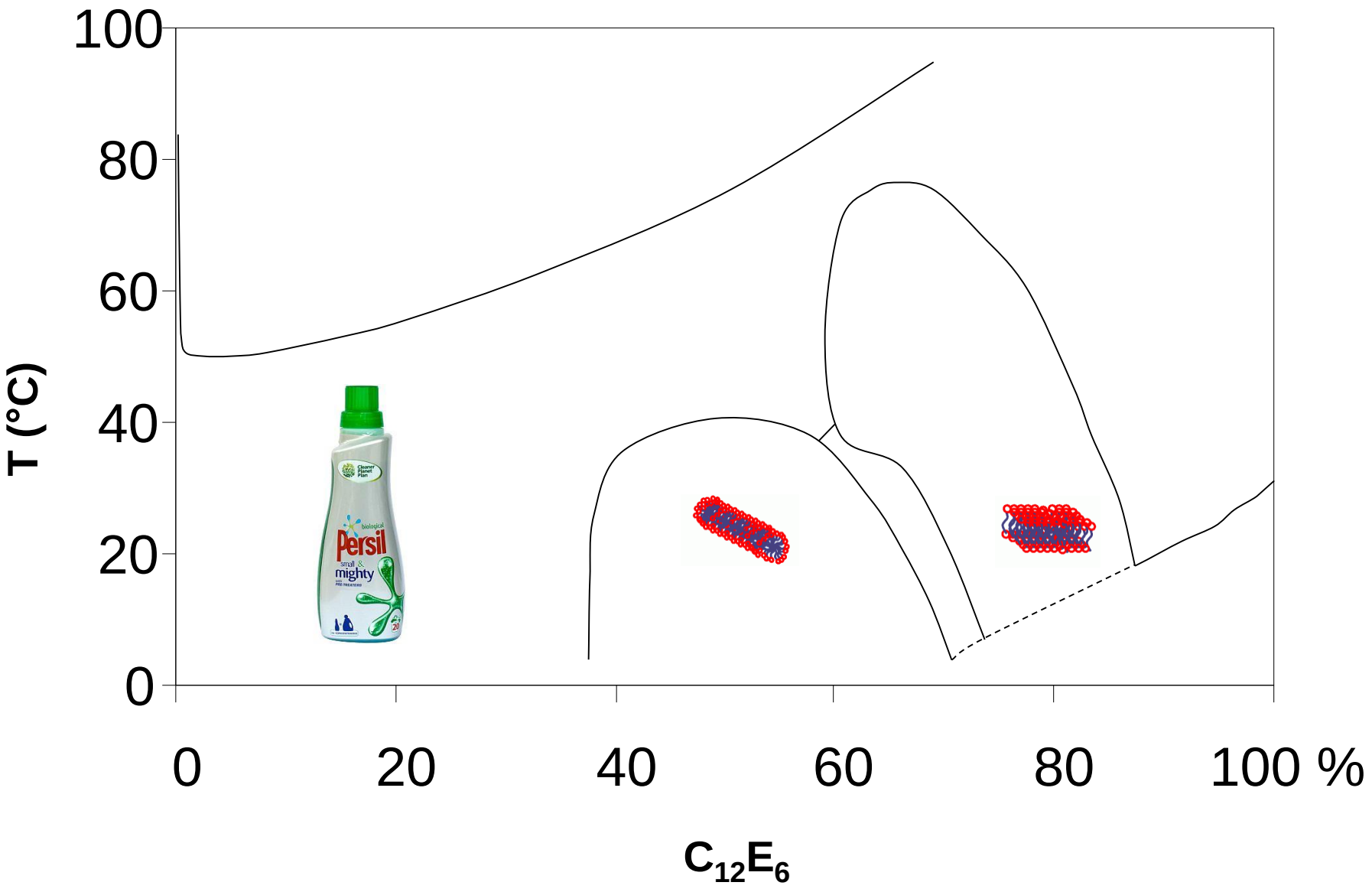


C_2 EO

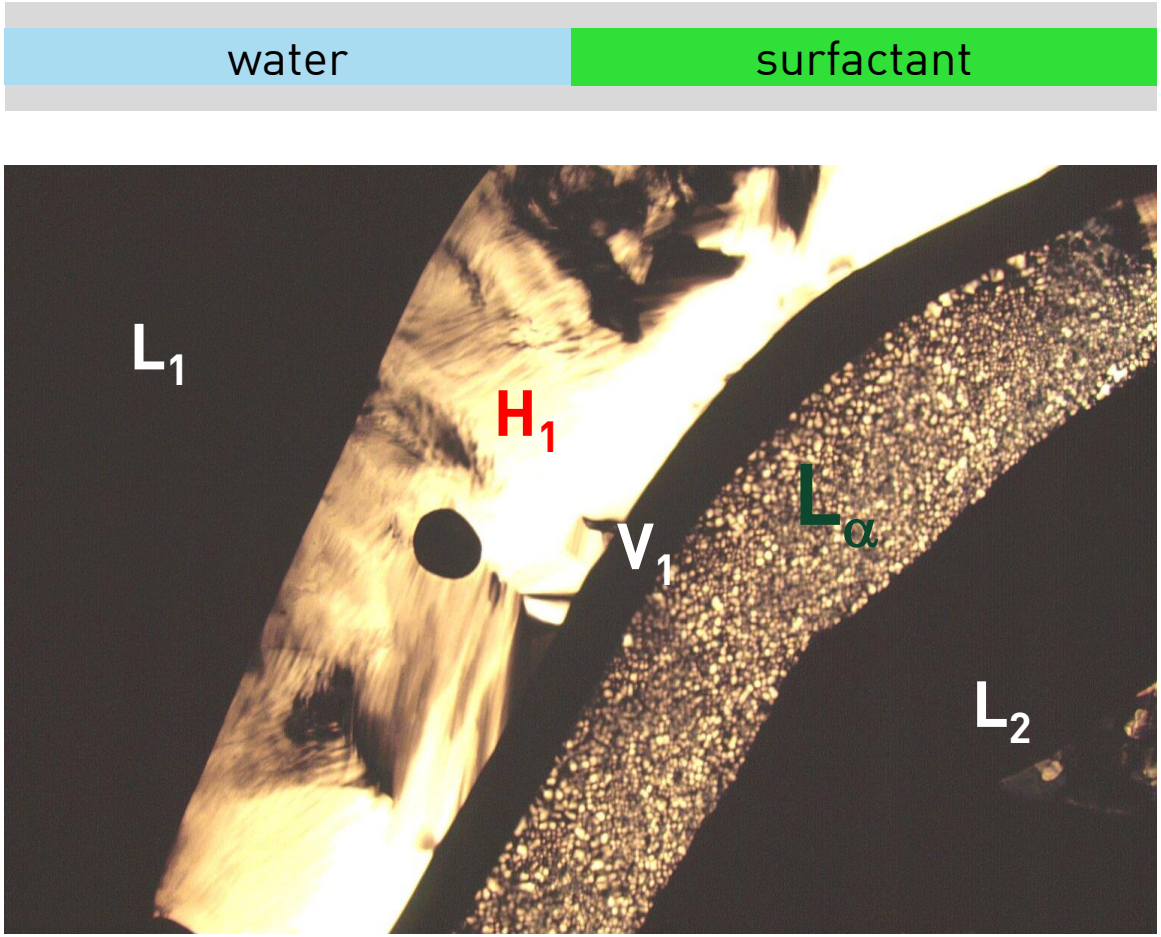




W


100
80
60
40
20
0
T (°C)
0
20
40
60
80
100 %
C12E6
Persil
biological
small & mighty

PENETRATION SCAN



L_1, V_1 and L_2 isotropic hence black in crossed polars

H_1 – characteristic texture

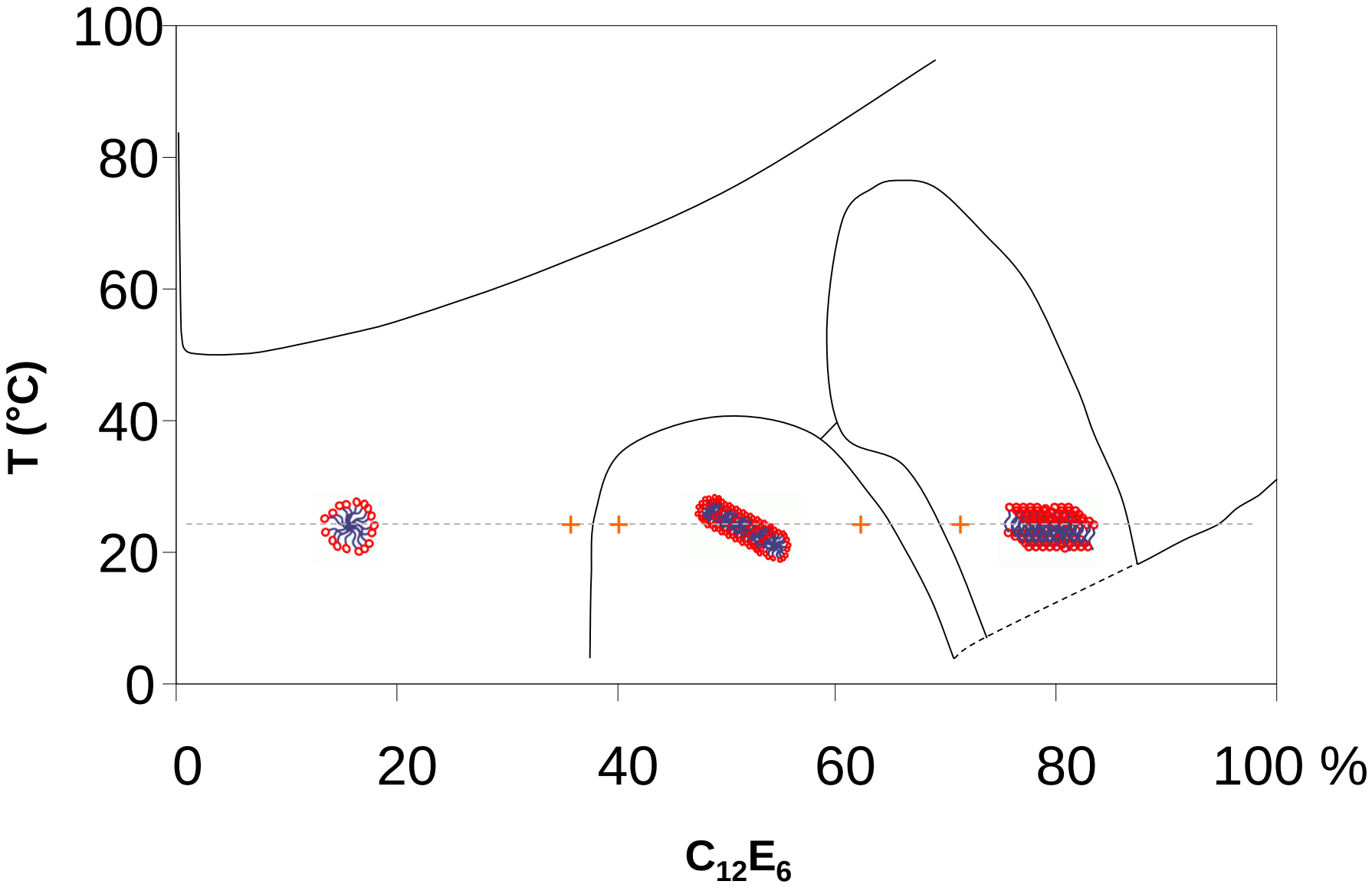
L_α – Maltese cross texture

Courtesy of Phil Moore, Unilever R&D Port Sunlight

PENETRATION SCAN "*IN-SILICO*"

Water	Surfactant

P. Prinsen, P. B. Warren and M. A. J. Michels, Phys. Rev. Lett. 89, 148302 (2002)


100
80
60
40
20
0
T (°C)
0
20
40
60
80
100 %
C12E6

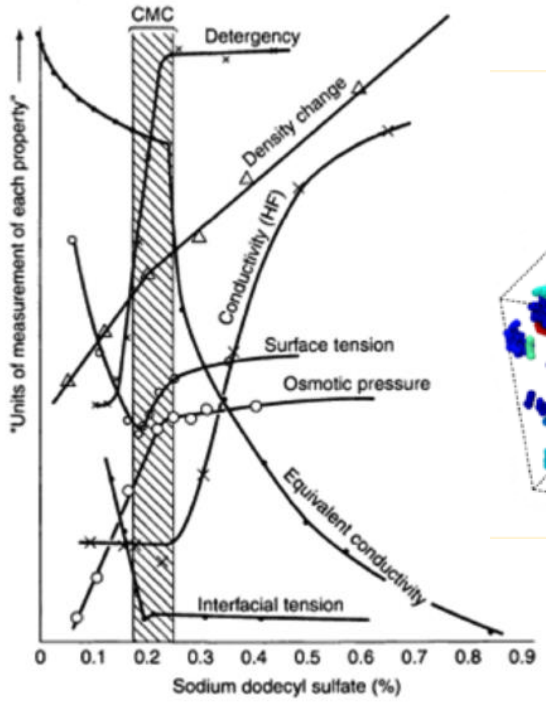
THE JOURNAL OF PHYSICAL CHEMISTRY B

Article

pubs.acs.org/JPCB

Toward a Standard Protocol for Micelle Simulation

Michael A. Johnston,[†] William C. Swope,*[,‡] Kirk E. Jordan,[§] Patrick B. Warren, Massimo G. Noro,[∥] David J. Bray,[⊥] and Richard L. Anderson*[,⊥]



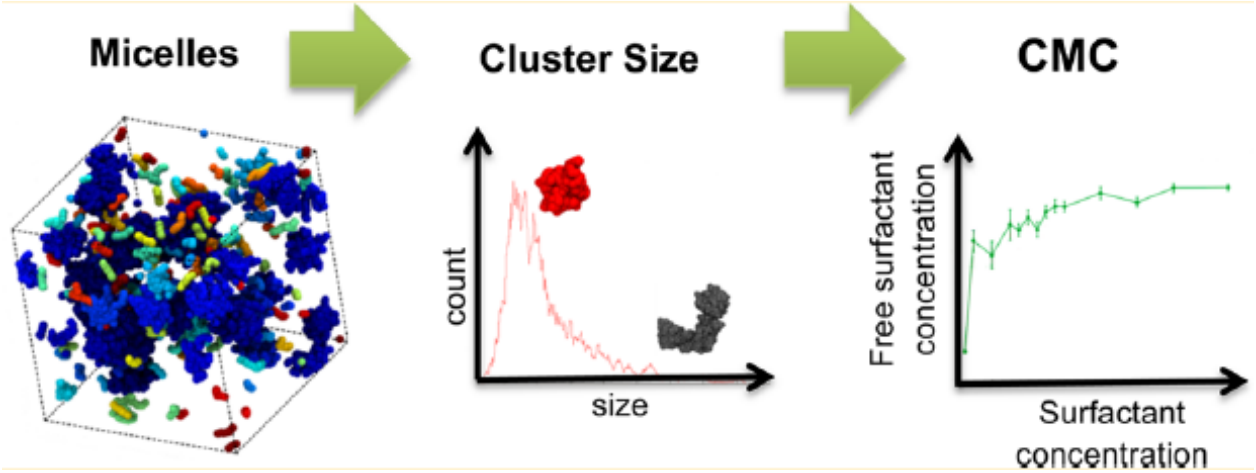
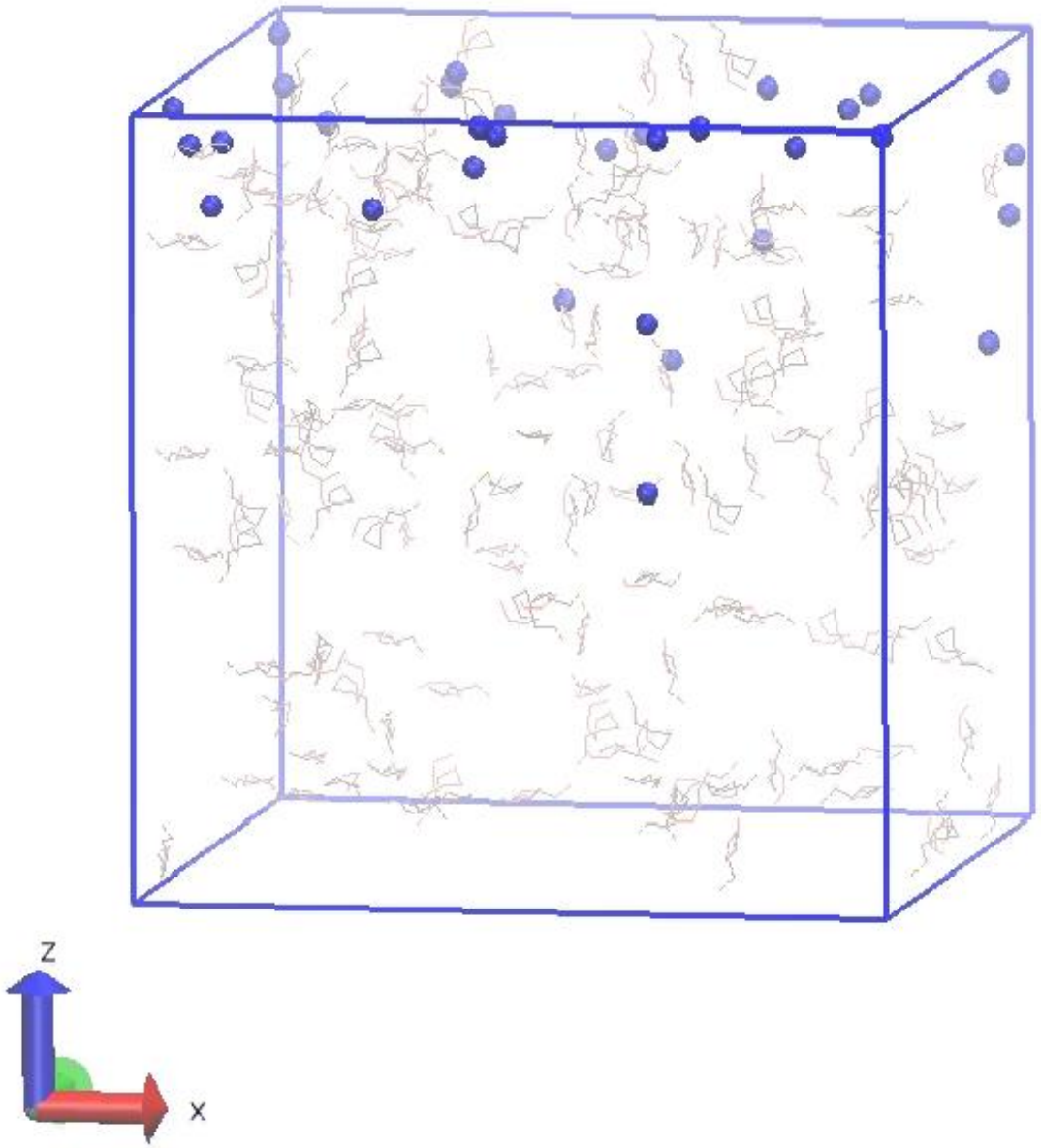
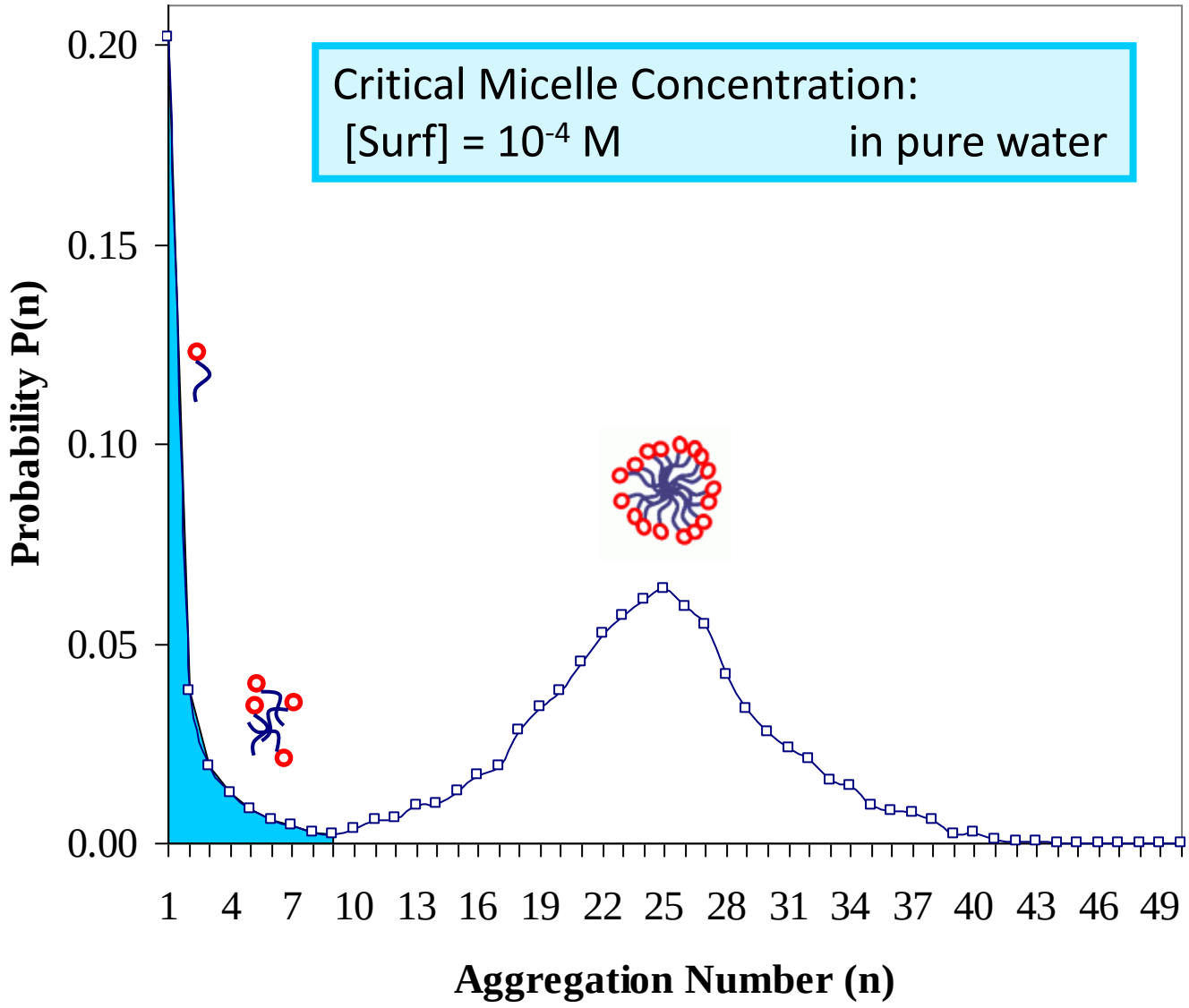


Figure 1. Changes in a number of physical properties for an aqueous solution of sodium dodecyl sulfate as the concentration of solution is increased from below to above the CMC. (Reprinted with permission from ref 10. Copyright 1948 American Chemical Society.)

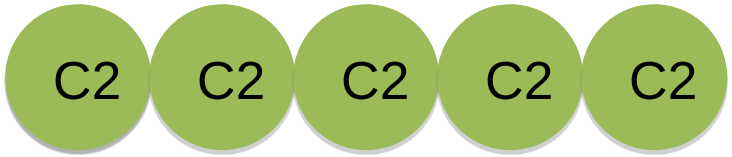

Z
X


Critical Micelle Concentration:
[Surf] = 10-4 M in pure water
Probability P(n)
0.20
0.15
0.10
0.05
0.00
1 4 7 10 13 16 19 22 25 28 31 34 37 40 43 46 49
Aggregation Number (n)

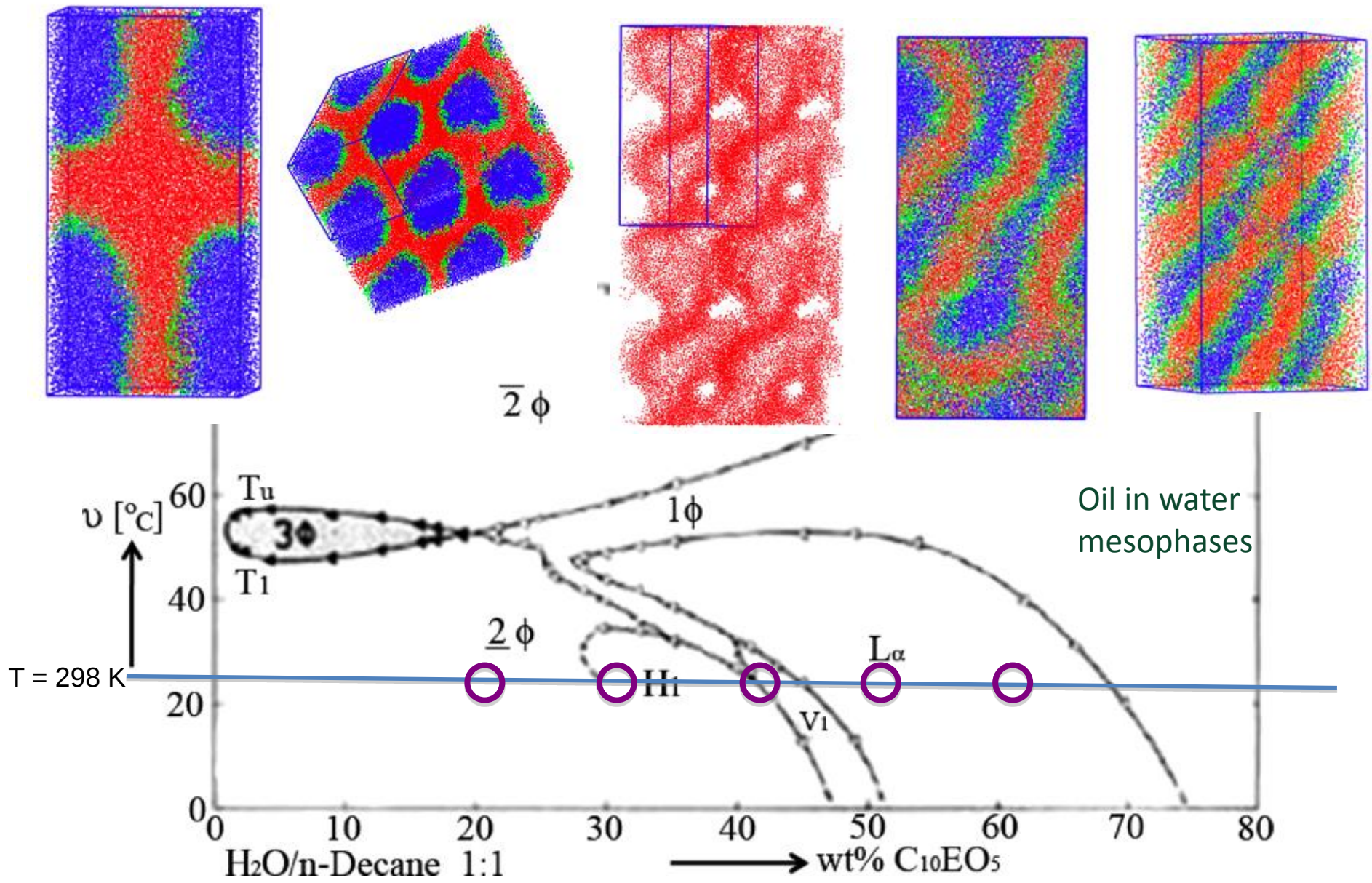
CLEANING AWAY THE OIL

= $C_{10}E_5$

= H_2O



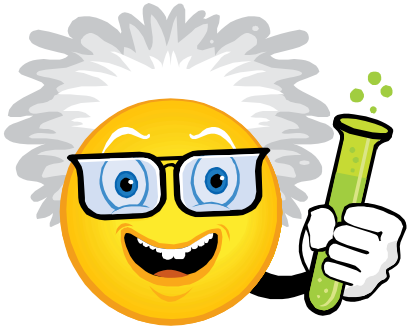
= Decane



R Dong and J Hao, Chem. Rev., 110, 4798 (2010)

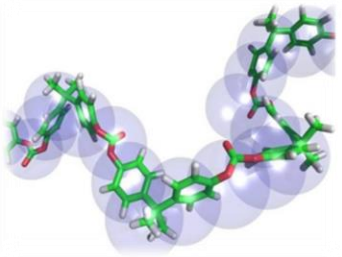
WHO IS THIS FOR ?

- Formulators (now and the future)



- Deliver capability to individual desktops & laptops

built a model for liquid mixtures



coded the interface with the BlueGene/Q

A powerful supercomputer on the palm of you hand

SUMMARY

1. Industrial challenges in surfactant science
2. Mesoscale computational approach
3. Applications:
    - phase behaviour
    - micellar properties
4. Deploying to end-users