COMPUTER AIDED FORMULATION (CAF): INDUSTRIAL NEEDS FOR CCP SAS

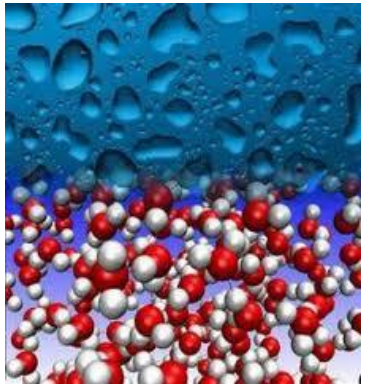
Pete Dowding, Principal Scientist, Infineum UK, Milton Hill

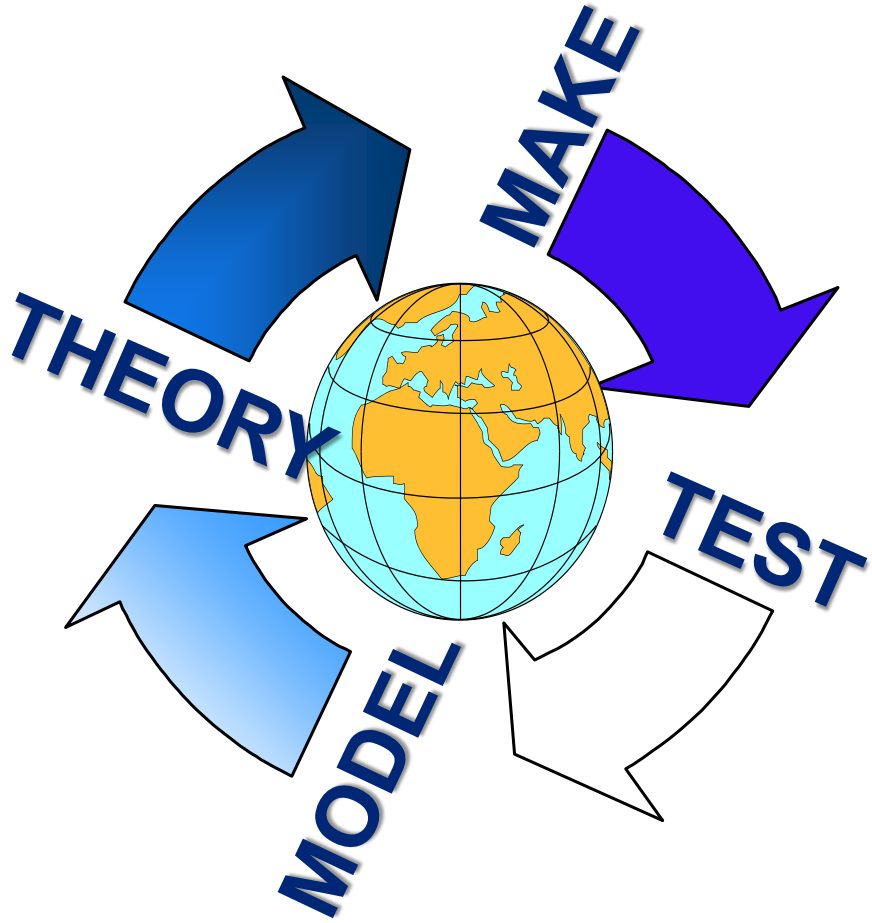
Performance you can rely on.

Infineum

© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved.

R&D Circle in Industry

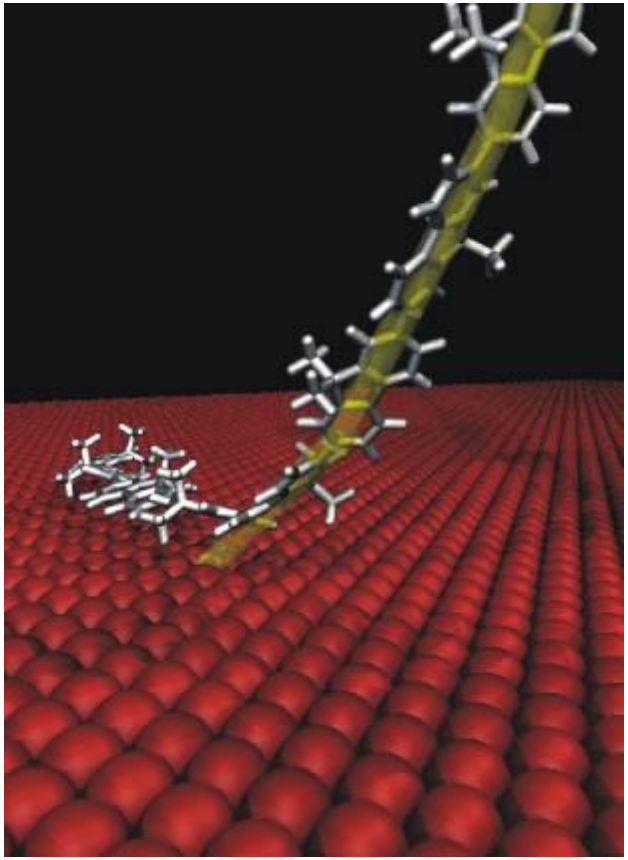




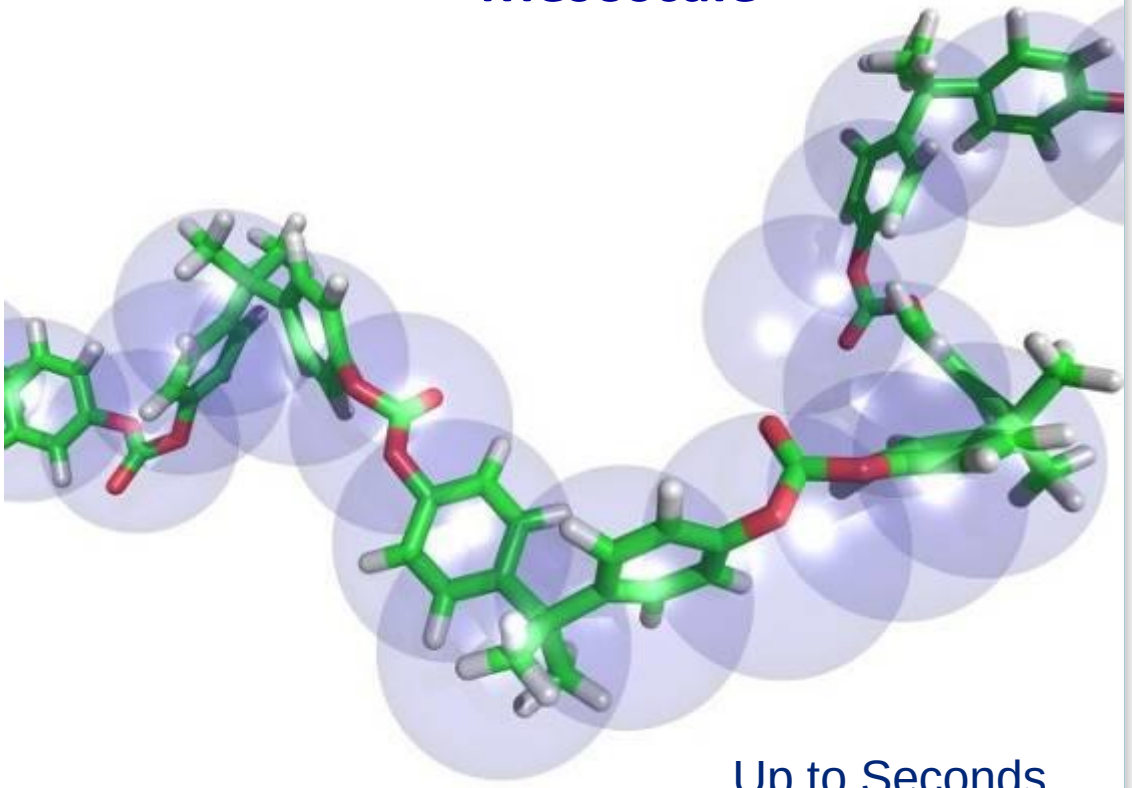
© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved.

Modelling at the Mesoscale

Atomistic ⟷ **Mesoscale**



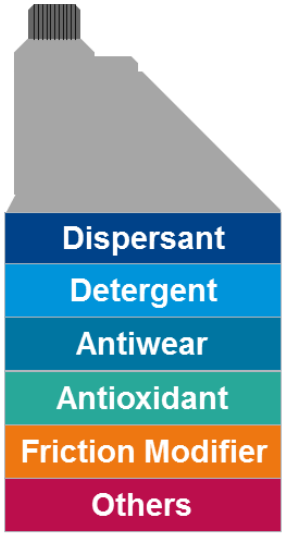
One millionth of a second (10^{-6}s)



Up to Seconds

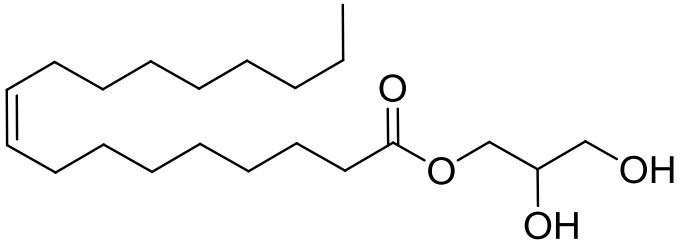
© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved.

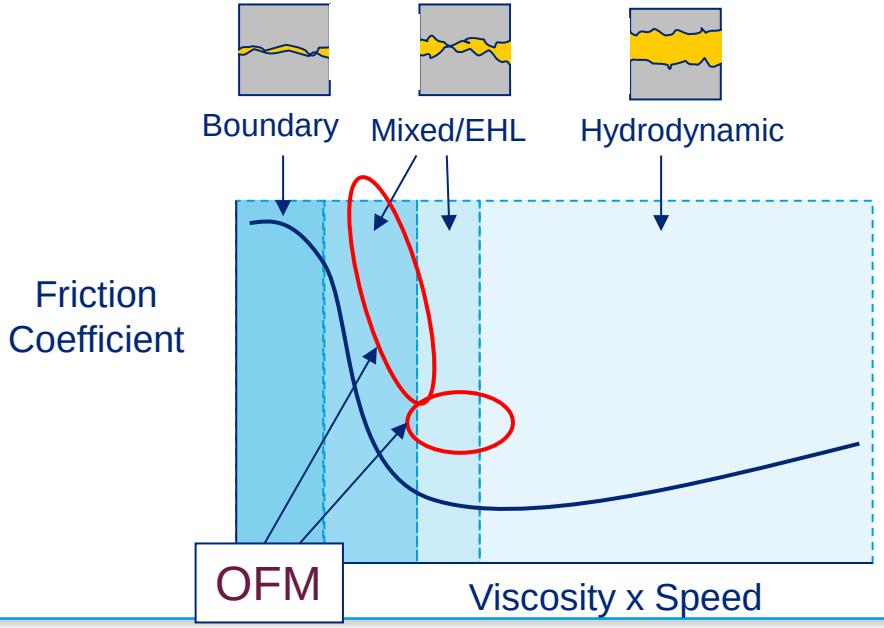
Industrial Systems: Lubricant Additives



- Vehicle lubricants comprise non-aqueous formulations of surfactants, polymers & particles
- Environment is the main driver, with fuel economy a key attribute
- The largest effect on fuel economy from the lubricant is based on viscosity but organic friction modifiers (OFM) have an effect

GMO



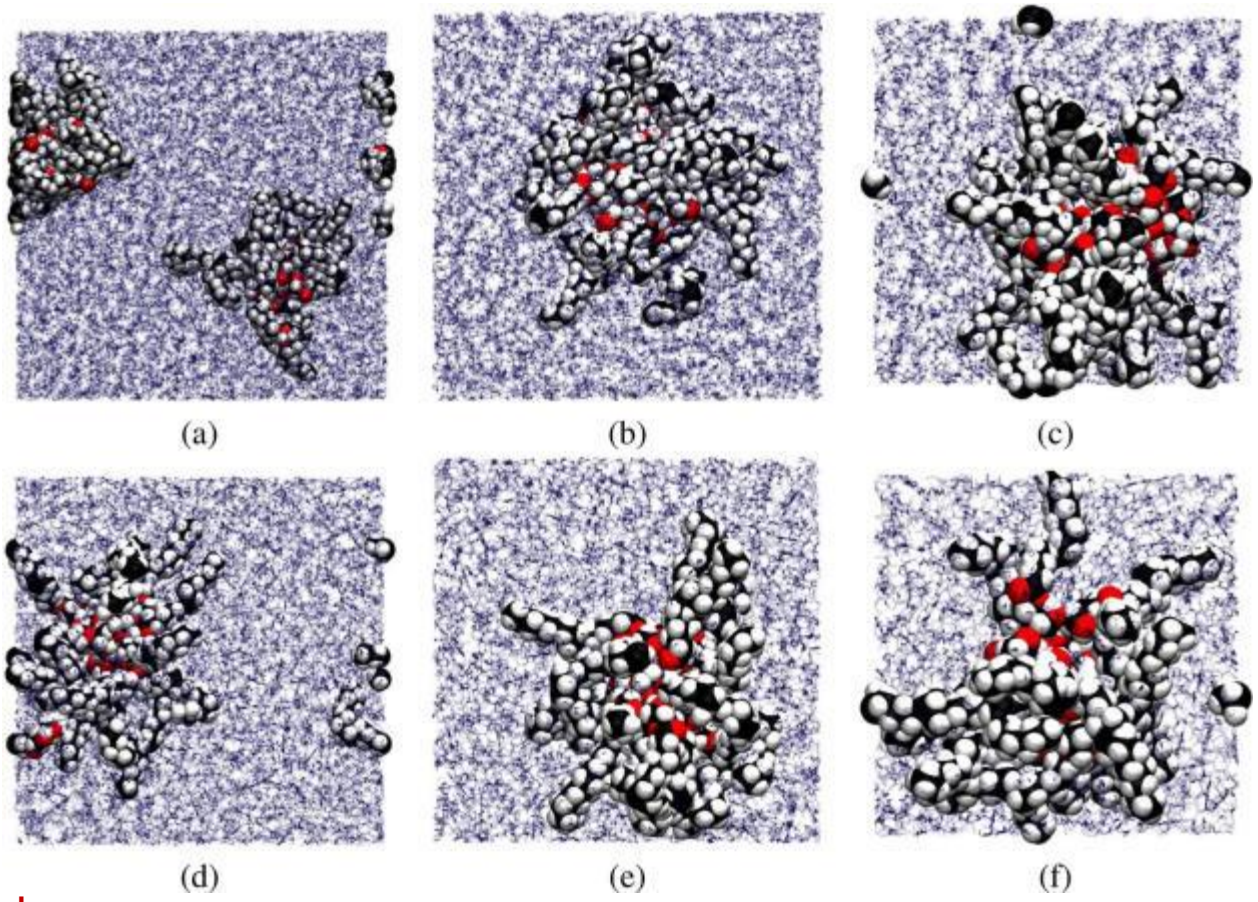


© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved.

MD simulation of Glycerol monooleate self-assembly in non-aqueous media

Increasing concentration (5-20%)

heptane



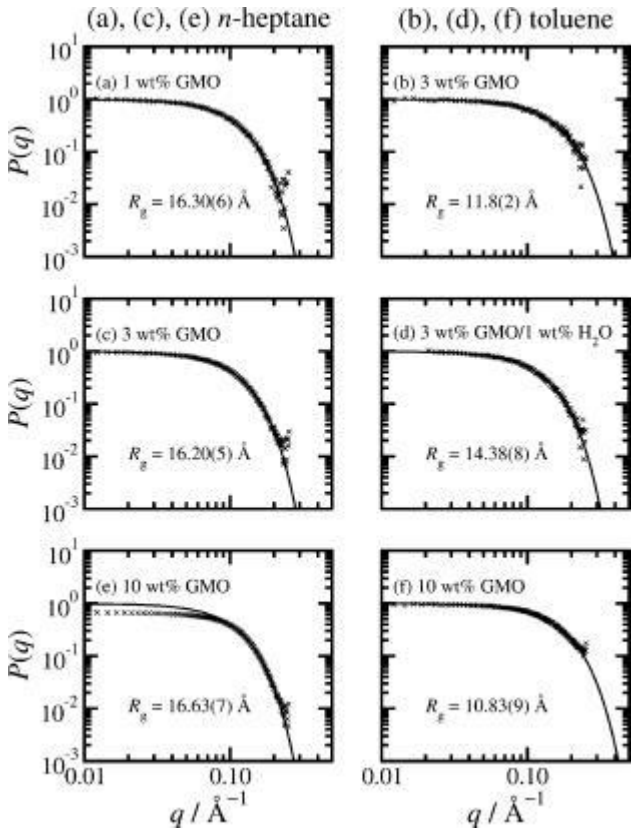
toluene

J. Phys. Chem. B 2015, 119, 4321−4331

© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved.

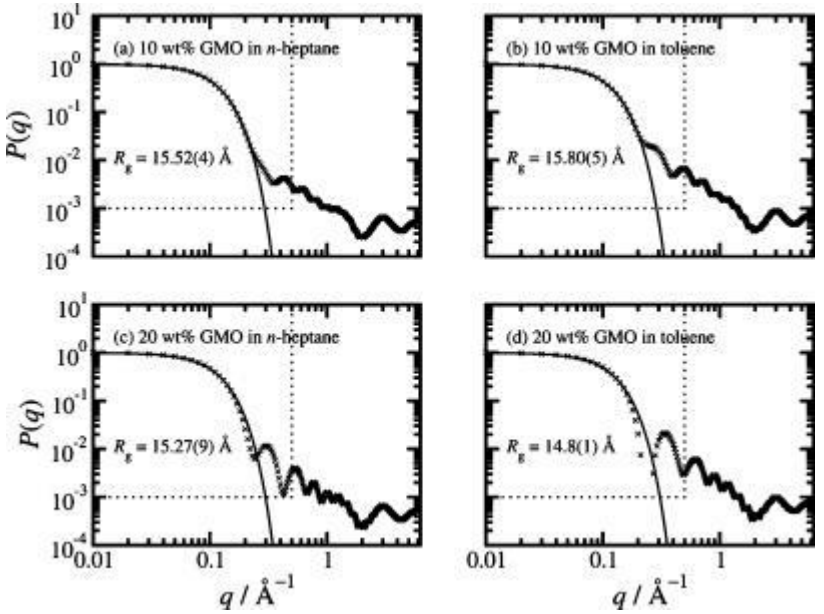
MD Simulation of SANS Profiles

- Experimental form factor from SANS measurements:



fits using Gaussian form factor

- Simulated form factor:



Future: Tools to simulate and rationalise scattering data (in real-time!) would be valuable

J. Phys. Chem. B 2015, 119, 4321−4331

© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved.

Computer Aided Formulation (CAF)

- Computer Aided Formulation (CAF) is a UK-Government funded (Innovate UK) collaborative research programme worth ~ £1.2 Million. Ended 31/5/17
- Partners:

Unilever

Infineum

syngenta

Novidec
Data Driven Decisions

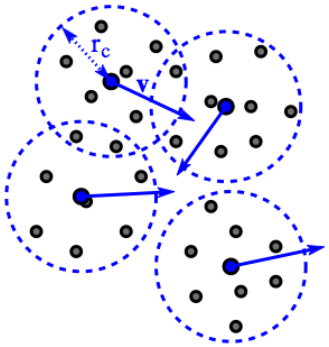
Science & Technology Facilities Council

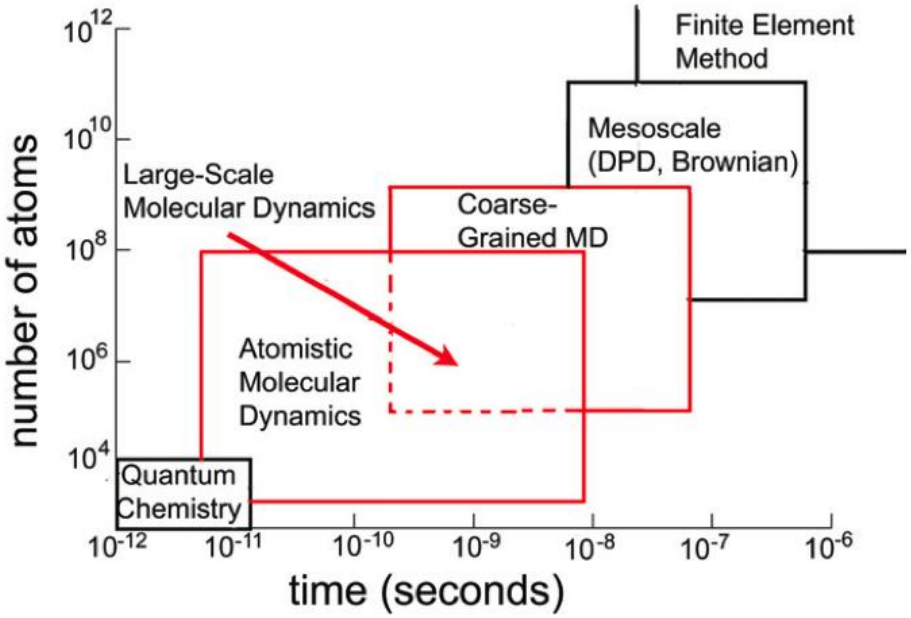
- *Aims:* Development of a new, fully automated method for optimizing the fit of dissipative particle dynamics interaction parameters to appropriate experimental data to predict phase diagrams, solubility parameters, CMC etc.
- This results in predictive modeling and simulation, to improve product formulation, accelerating the development of new products.

© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved.

Coarse Grain Modelling

- Mesoscopic simulation method
- Developed by Hoogerbrugge and Koelman (1992)
- Coarse-grained method



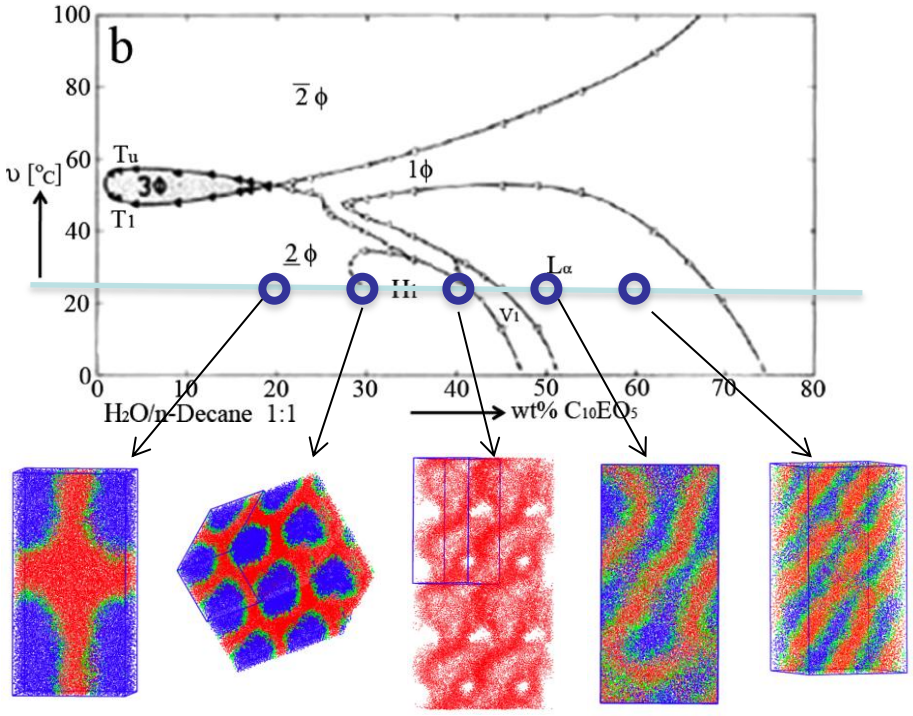


- Access to longer length and time scales compared to fully atomistic methods.
- Simulation platform based on open source (STFC) DL_MESO software

© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved.

Application of Predictive Coarse Grain Modelling

- Winsor's Fish for C_nEO_m



Composition Wt % $C_{10}E_5$	Expected Phase	SDPD Parameters
20	2Φ	2Φ
30	H_1	H_1
40	H_1/V_1	V_1
50	L_α	L_α (poorly ordered)
60	L_α	L_α (well ordered)

- CAF/ DPD Model has correctly predicted composition of phases

© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved.

Relevance to CCP-SAS for the future

- There has been discussion regarding simulation/ prediction of SANS data using DPD/ coarse graining, but no development work has been done during CAF
- Fitting such data takes considerable time and is generally performed post-experiment
- What if there was an algorithm that would take the output of soft-matter computer simulation to predict both the SANS and the SAXS spectra
- An algorithm to solve the inverse problem too: from SANS and SAXS spectra that would predict the corresponding soft-matter configuration without user bias in the fit eventually extending to complex mixtures (formulations)
- Development of such tools would be of real value to industry- towards the Nirvana of data being fitted as it is generated to make smarter decisions in real-time during the experiment
- Also allows non-expert users to perform structural characterisation

© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved.

Permission is given for storage of one copy in electronic means for reference purposes. Further reproduction of any material is prohibited without prior written consent of Infineum International Limited. The information contained in this document is based upon data believed to be reliable at the time of going to press and relates only to the matters specifically mentioned in this document. Although Infineum has used reasonable skill and care in the preparation of this information, in the absence of any overriding obligations arising under a specific contract, no representation, warranty (express or implied), or guarantee is made as to the suitability, accuracy, reliability or completeness of the information; nothing in this document shall reduce the user's responsibility to satisfy itself as to the suitability, accuracy, reliability, and completeness of such information for its particular use; there is no warranty against intellectual property infringement; and Infineum shall not be liable for any loss, damage or injury that may occur from the use of this information other than death or personal injury caused by its negligence. No statement shall be construed as an endorsement of any product or process. For greater certainty, before use of information contained in this document, particularly if the product is used for a purpose or under conditions which are abnormal or not reasonably foreseeable, this information must be reviewed with the supplier of such information.

Links to third party websites from this document are provided solely for your convenience. Infineum does not control and is not responsible for the content of those third party websites. If you decide to access any of those websites, you do so entirely at your own risk. Please also refer to our Privacy Policy.

© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved.

"INFINEUM, PARATAC, SYNACTO, VISTONE and the interlocking ripple device are Trade Marks of Infineum International Limited

© INFINEUM INTERNATIONAL LIMITED 2016. All rights reserved. Infineum Confidential