Combining molecular dynamic simulation with neutron reflectometry to understand and predict friction

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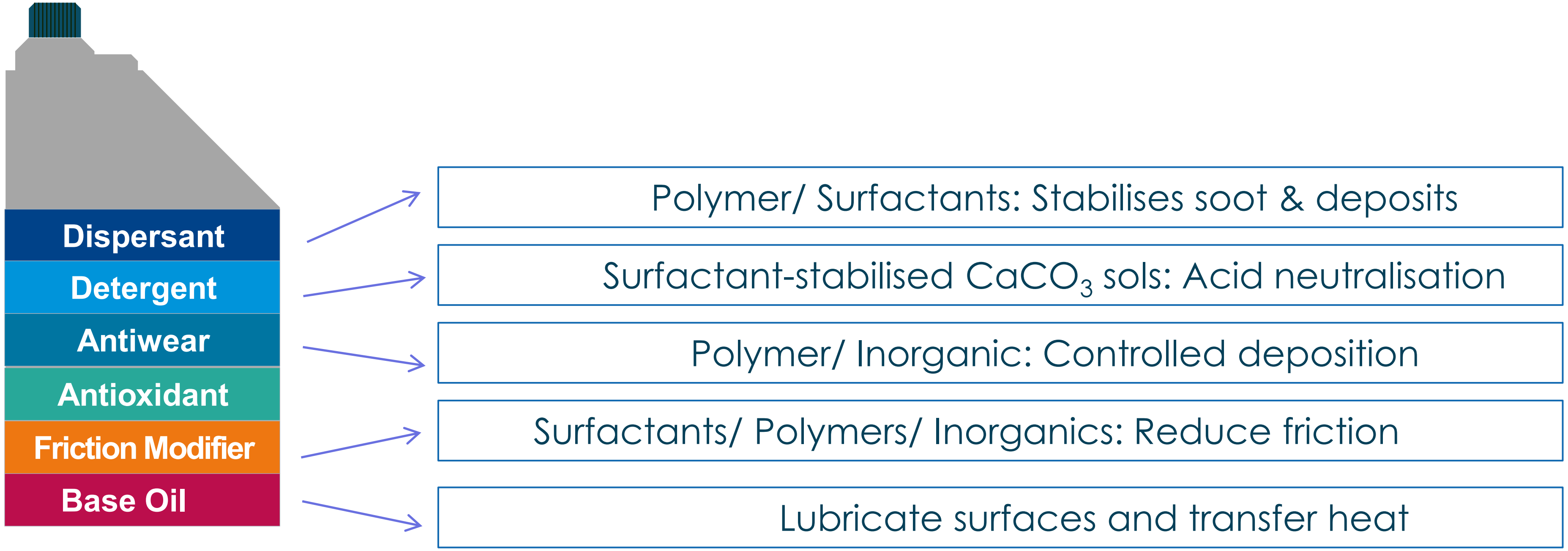
Lubricant Additives

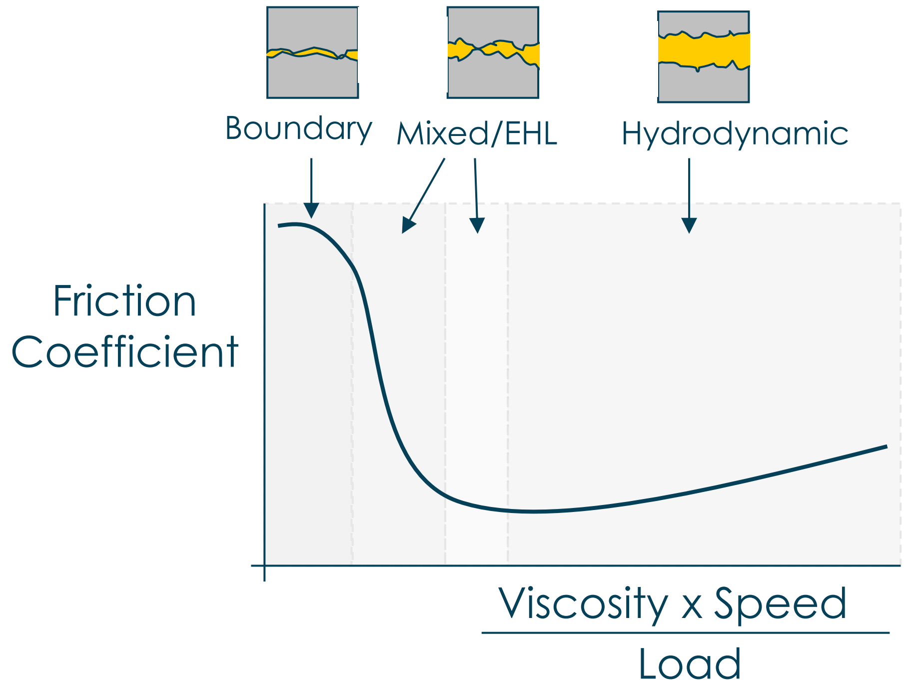
- Lubricants can contain up to 10 different additives, dependent upon application (cars are different to trucks and very different to ships)



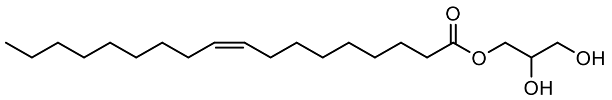
- Environment drives base-business research:
  - *Improved fuel* economy: Reduced emissions: a 5% improvement in fuel economy would lead to a reduction of ~50 MT/ year CO_2 emissions globally
  - 20–25% of global energy is lost to friction: 7 Billion tonnes of CO_2 emitted per year overcoming friction: relevant to electric vehicles, wind turbines etc.

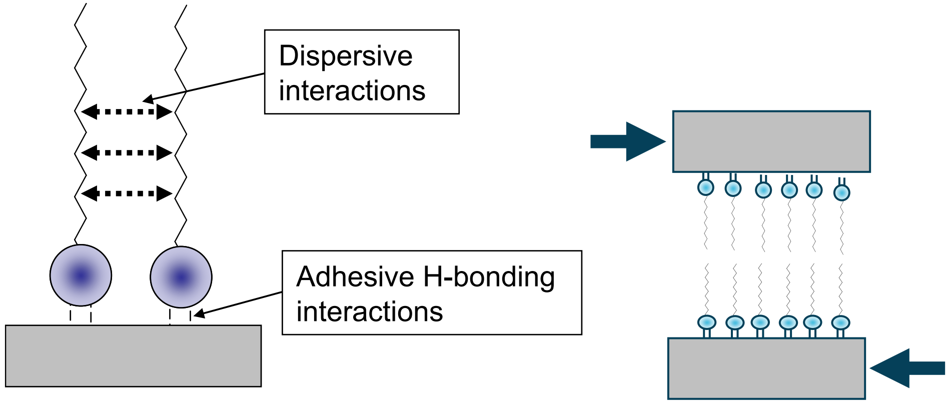
Improving Fuel Economy: Organic Friction Modifiers

- Fuel economy is the major driver in lubricants
- The largest effect on fuel economy from the lubricant is based on viscosity
- Friction modifiers reduce friction and hence improve fuel economy



Glycerol monooleate (GMO)

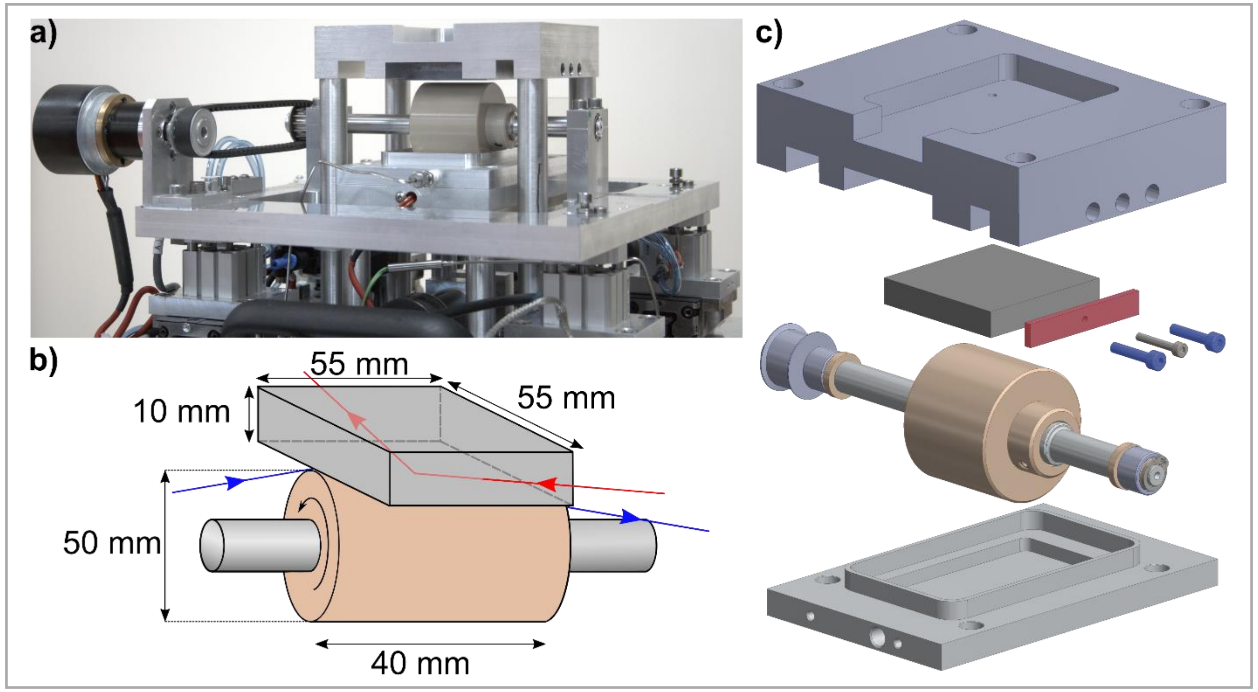




- What is the mode of action for organic friction modifiers?

  Published results: a monolayer with a slip-plane between head-group & surface

Beamline Tribometer

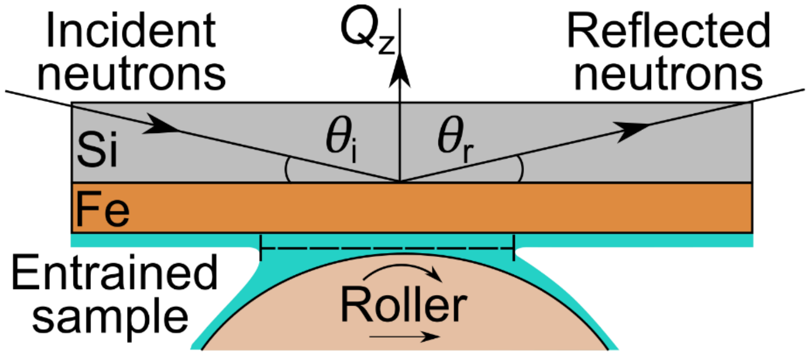


Blue = X-ray beam path
Red = Neutron beam path

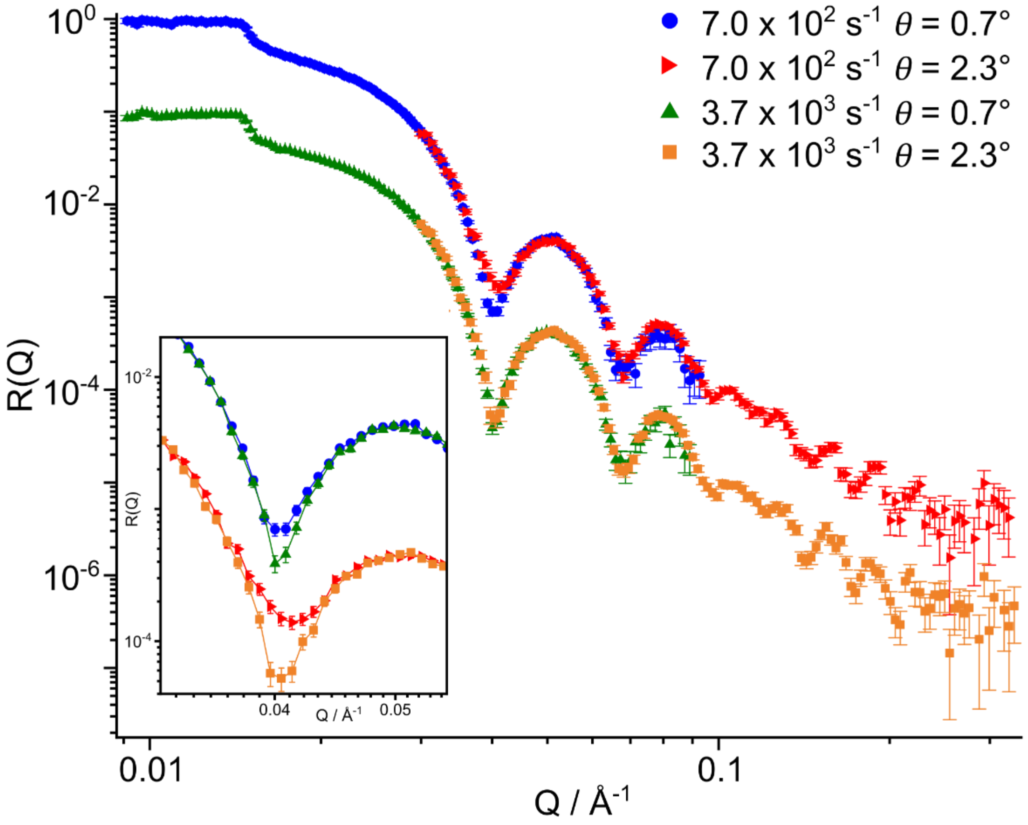
- Provides shear to solid-liquid interface for in-situ X-ray/neutron reflectometry
- Loaded contact between roller & substrate or form a calibrated gap.

Experiment with dodecane-d_{26}

- Roller/substrate gap = 200 μm.
- Solvent entrained onto substrate at two different shear rate.
- Dodecane-d26 used as a model d-base oil (non-polar)



- Fringes arise from thickness of iron/iron oxide film



Entrained GMO/dodecane-d_{26} at the interface

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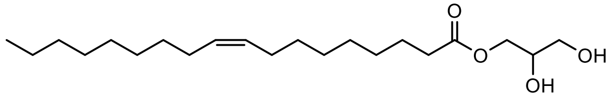
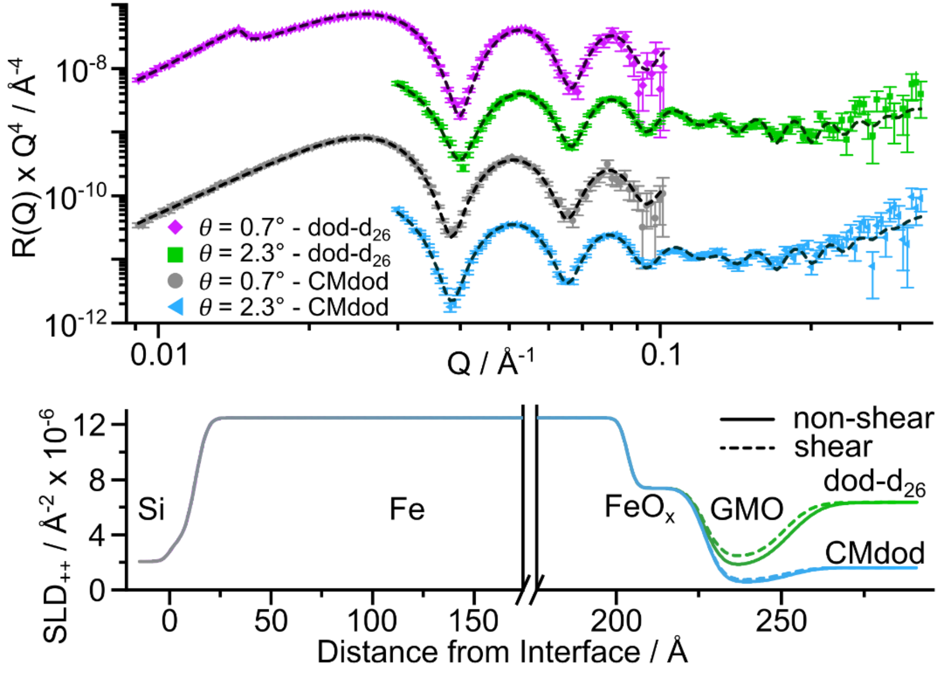
Glycerol monooleate (GMO)



Layer	SLD$_n$ / Å^{-2} × 10^{-6}	SLD$_m$ / Å^{-2} × 10^{-6}	Thickness / Å	Roughness / Å	Solvation / %
Si	2.07	-	∞	3.0	-
SiO$_2$	3.47	-	$12.7^{+2.9}_{-7.4}$	$4.6^{+1.9}_{-3.6}$	-
Fe	$7.9^{+0.1}_{-0.1}$	$4.6^{+0.2}_{-0.2}$	$19.1^{+0.1}_{-0.2}\times10^{1}$	$2.1^{+4.4}_{-1.1}$	-
FeO$_x$	$6.9^{+0.3}_{-0.3}$	$0.5^{+0.3}_{-0.3}$	$23.3^{+0.8}_{-0.8}$	$4.3^{+4.8}_{-2.3}$	-
†GMO	0.21	-	$24.3^{+9.9}_{-10.2}$	$6.7^{+3.3}_{-4.7}$	$35.2^{+45.3}_{-35.2}$
‡GMO	0.21	-	$25.8^{+4.4}_{-5.2}$	$7.7^{+2.3}_{-5.7}$	$24.5^{+21.6}_{-22.4}$

- Fitted thicknesses of GMO could suggest more complex structures than monolayer.



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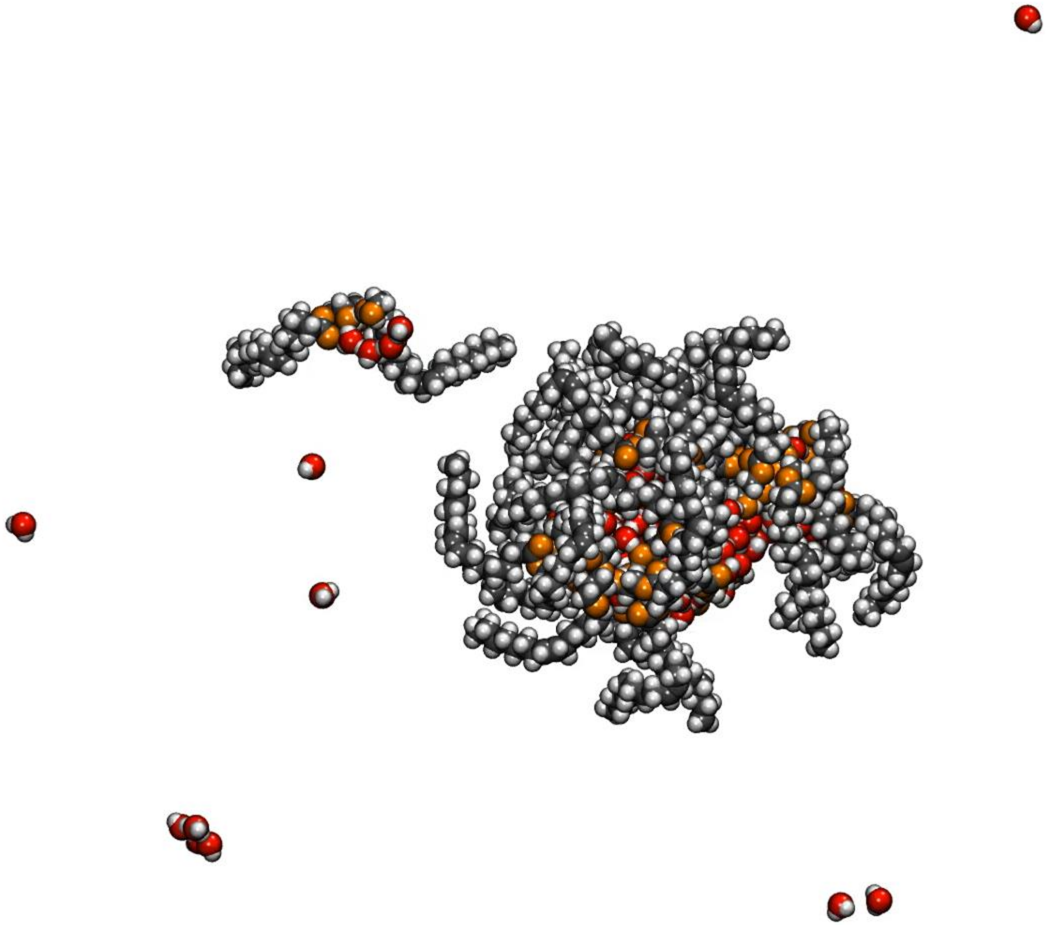
G. Tsagkaropoulou, C. P. Warrens and P. J. Camp, *ACS Appl. Mater. Interfaces*, 2019, **11**, 28359–28369

Computational Simulation by MD: Bulk GMO/water

- System properties
- 30 GMO molecules
- 1400 n-dodecane molecules
- 150 water molecules (5:1 water:GMO)
- T = 298.15K

- Results
- Reverse micelle with coordination number of 29
- $R_{\mathrm{g}} = 16.8 \pm 0.2$ Å

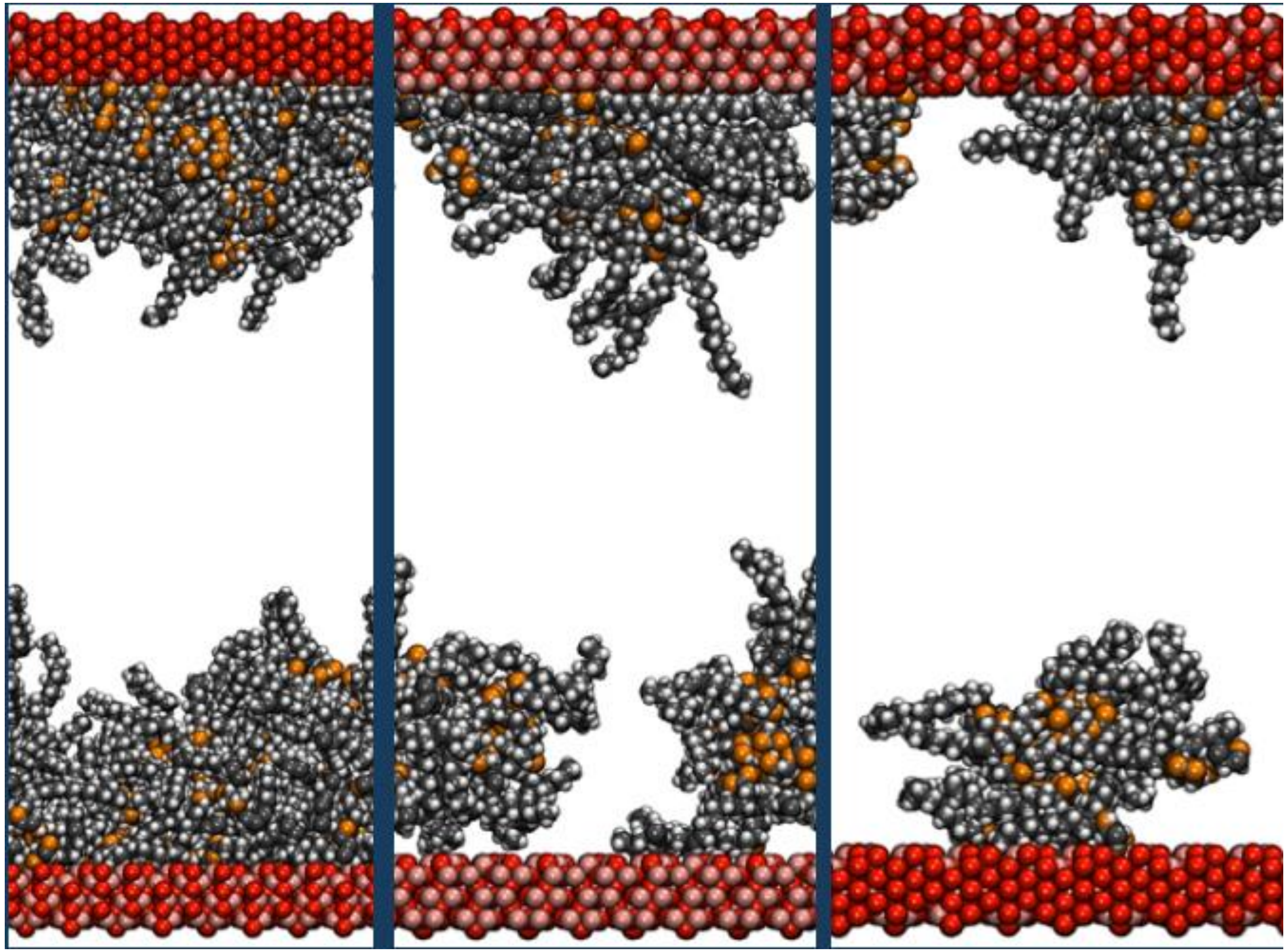


Confined GMO

- System properties:
- 156, 78, and 39 GMO molecules
- 589 n-dodecane molecules
- Two $55.088 \times 50.38 \times 8.61$ Å iron oxide surfaces
- T = 298.15K

- Observations:
- Prevalence of RM formation

- Friction coefficient:
  $\mu = 0.13$ @ $4 \times 10^{10}\ s^{-1}$

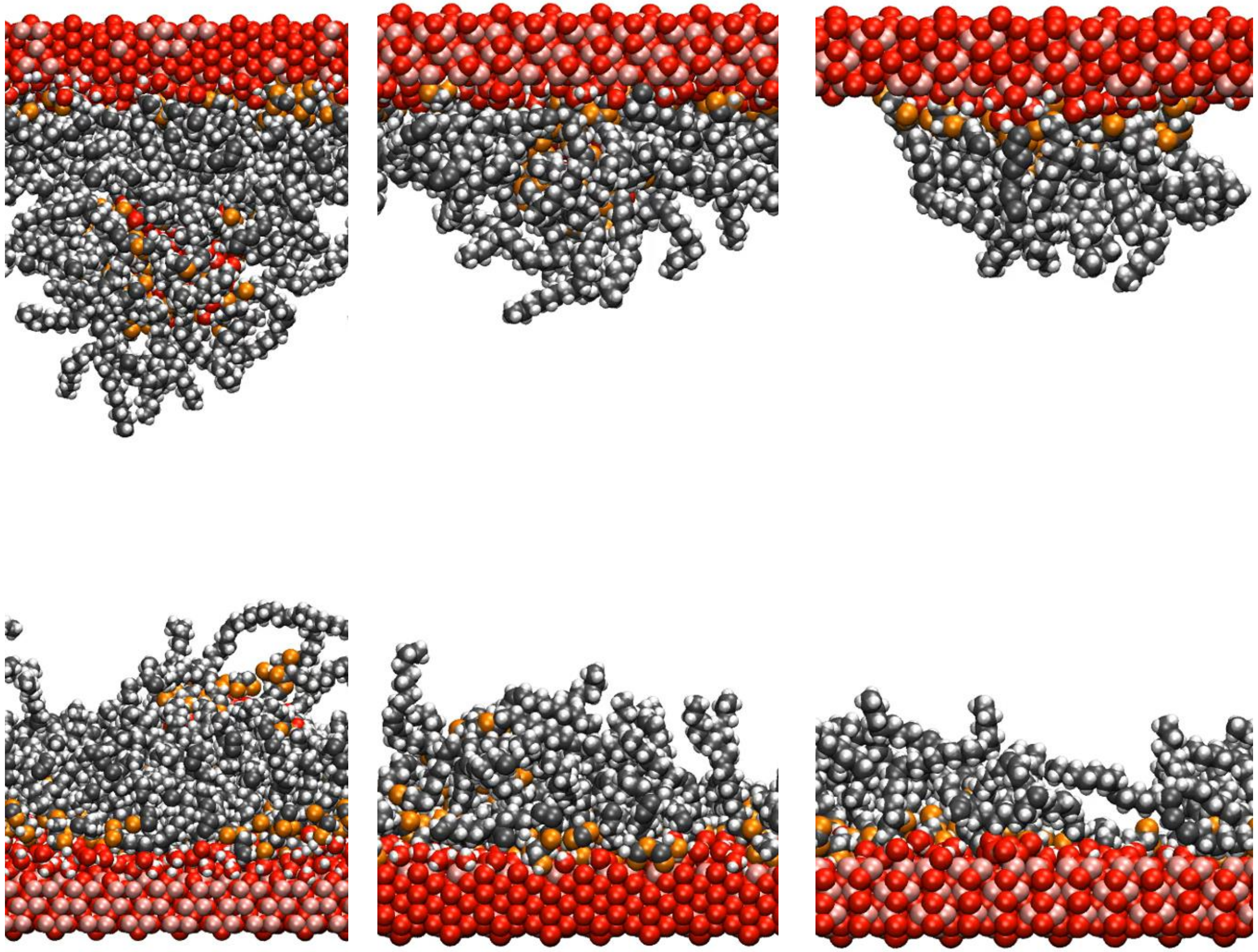


Confined GMO/ water

- System properties
- 174, 88, and 44 GMO molecules
- 589 n-dodecane molecules
- 5:1 water: GMO
- Two $55.088 \times 50.38 \times 8.61$ Å iron oxide surfaces
- T = 298.15K

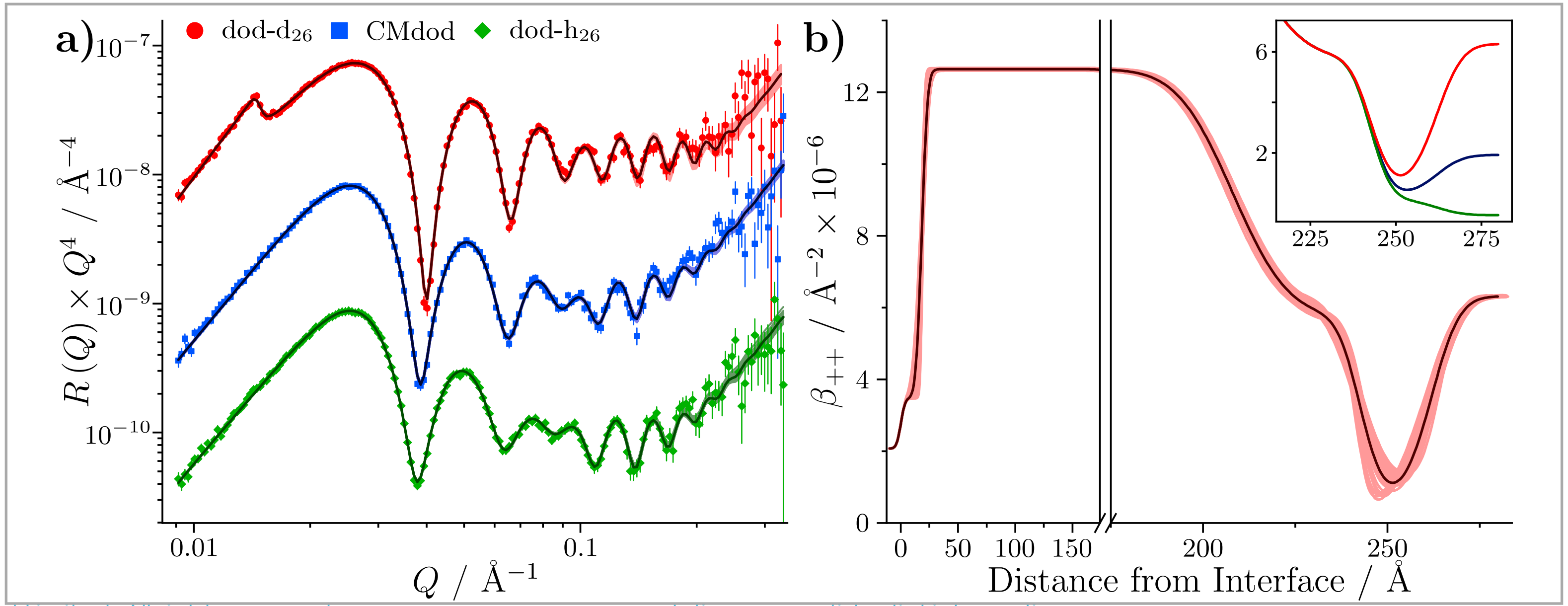
- Friction coefficient:
  μ = 0.16 @ 4 x 10^{10} s^{-1}

- Large water presence near surfaces, and more evidence of 'mono-layer' formation: highlights the importance of micelles structure and water content



MD Simulation of the SLD profile for neutron reflection

- Reflectivity of 20 mM GMO in dodecane against Fe-coated Si substrate in solid-liquid cell @ 25 °C.
- Thickness of GMO layer = $19.4^{+1.8}_{-1.6}$ Å
- Surface excess = $4.7^{+0.1}_{-0.1}$ mol m-2 x 10-6, APM = $35.5^{+1.0}_{-1.0}$ Å^2. Isotherms suggest APM = 40.0 ± 1.0 Å^2 (30 °C).
- Next step: Simulation calculates friction as a predictive tool



Conclusions & Acknowledgments

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- Neutrons can provide powerful structural insight into industrial products from the atomistic to macro scale

- Studies can be performed on [non-ideal] Industrial systems to unlock mechanistic and dynamic information

- Beamline tribometer: can now provide nano-scale structural measurements for systems in hydrodynamic and into mixed lubrication regimes:
  - Beamline tribometer can perform experiments in real-time
  - Results suggest that friction modifiers form more complex structures than a monolayer

- Computational Simulation: MD model successfully represents tribo-regimes found in the tribometer and can determine behaviour down to individual atoms.

- Next Steps: Apply to other areas where friction is relevant: fluids for electric vehicles, magnetorheological fluids, laundry, personal care etc.

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