

Small is Big in Tribology

University of Bath Research Day

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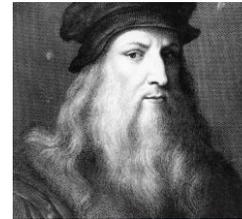
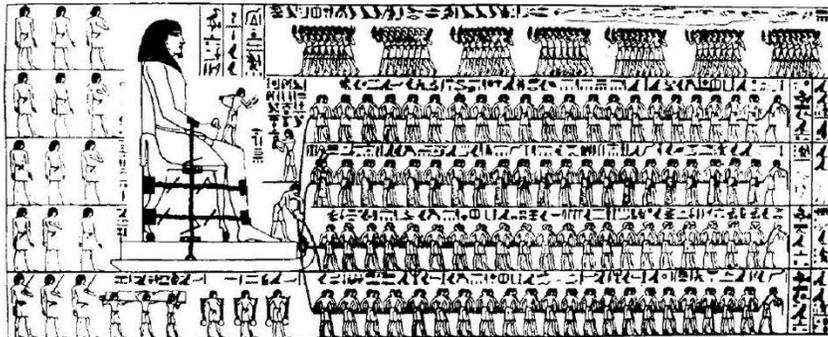
Introduction to Tribology

“Tribology is the study of interacting sliding surfaces.
It includes three subjects: friction, wear, and lubrication.”

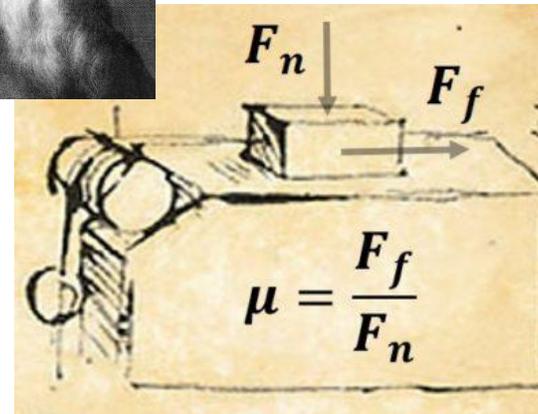
Encyclopaedia Britannica

“the most important subject no one has heard of”
New Scientist

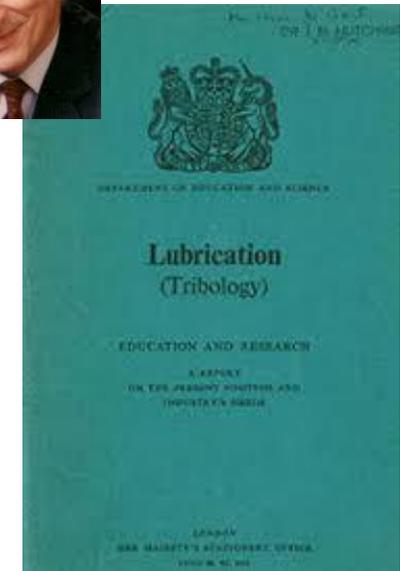
Ancient Egypt
~1880 BC



Leonardo Da Vinci
~1493 AD



1966



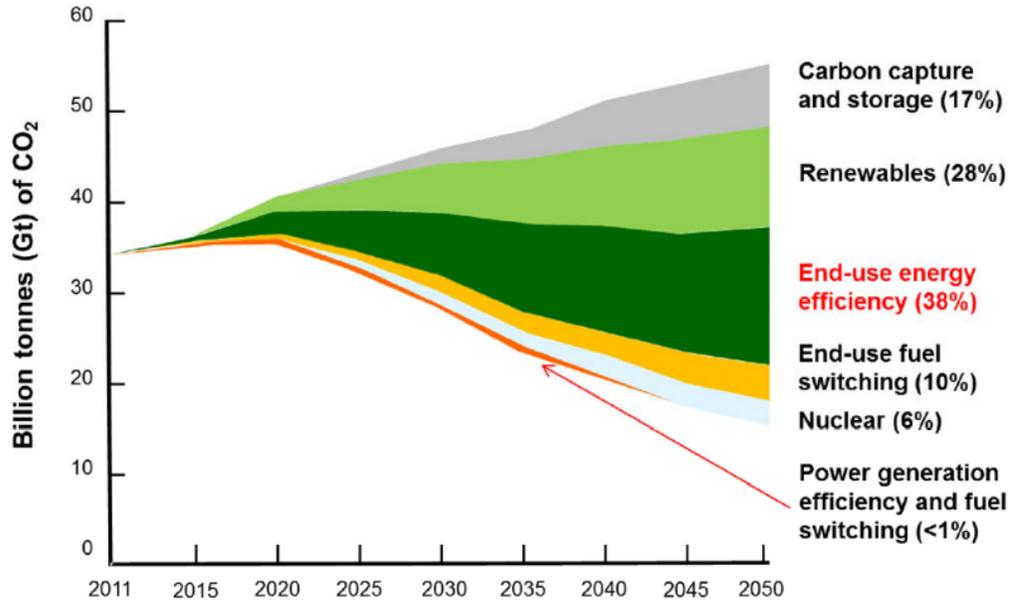
Guillaume Amontons
1699

Nosonovsky *Tribol. Online* **2**, 44-49 (2007)

Hutchings *Wear*. **360**, 51-66 (2016)

1.1-1.4 % of UK GDP
Williams Lubricants. **12**, 65 (2024)

Tribology and Energy Efficiency



Solid Lubricants

Aerospace



Ref.: *Energy Technology Perspectives 2014, Paris, OECD/IEA*

Table 1 Comparison of energy and costs due to friction and wear for the four economic sectors.

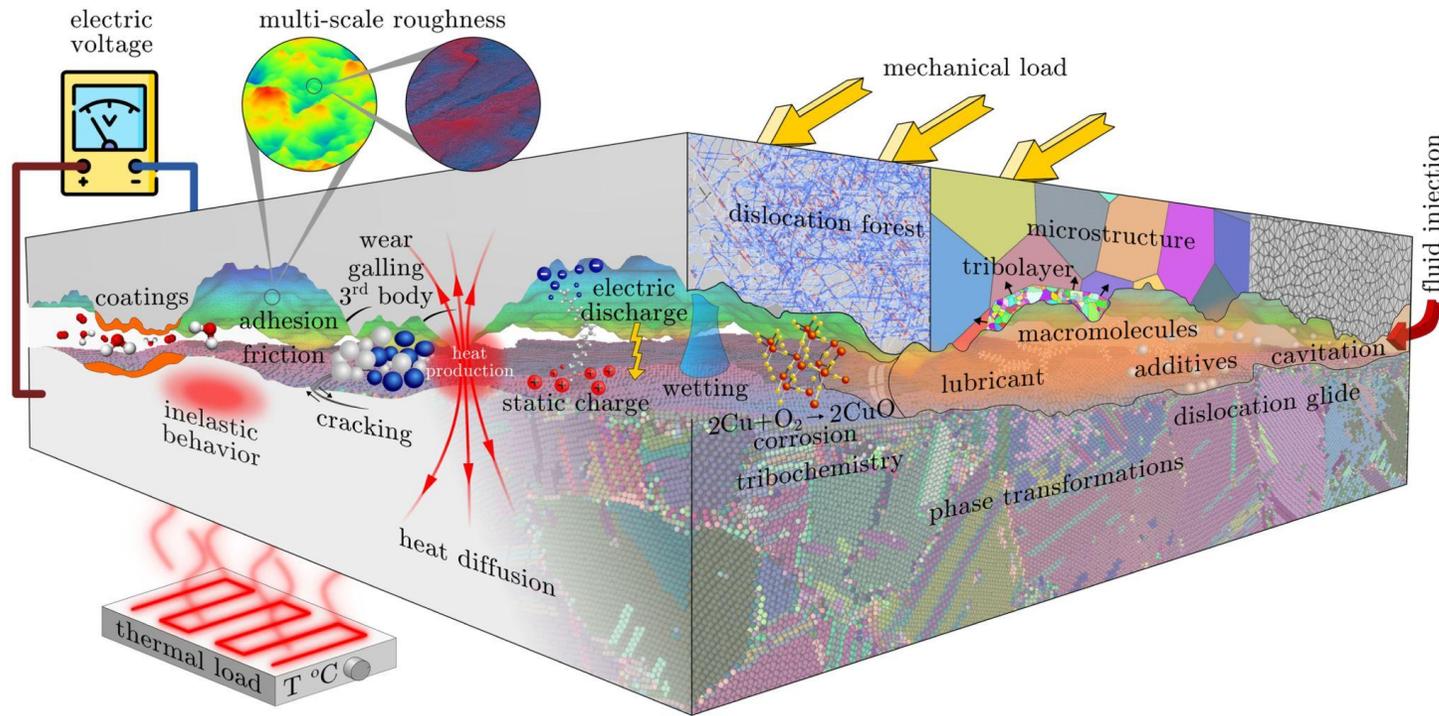
	Energy to overcome friction as part of total energy use	Energy due to wear compared to energy loss due to friction	Costs due to wear compared to costs due to friction
Unit	%	%	%
Transportation	30	10	22
Industry	20	14	35
Energy industry	20	22	53
Residential	10	14	35
Total	20	15	37

Particle Accelerators

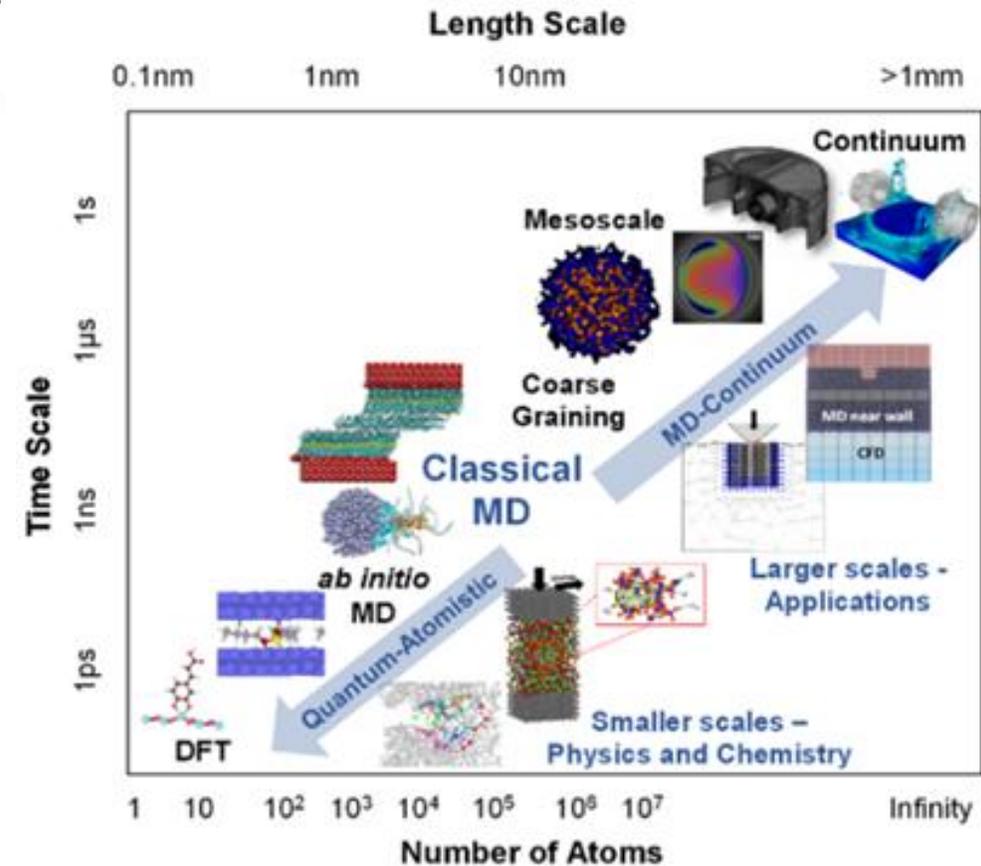


Grützmacher et al. *Adv. Mater.* **38**, e00867 (2026)

Modelling in Tribology



Pastewka, ..., Ewen, et al. *Tribol. Int.* **218**, 111326 (2026)



Ewen et al. *Friction.* **6**, 349-386 (2018)

Molecular Dynamics

- MD utilises Newton's equations of motion (EoM)
- EoM solved to determine trajectories for a system of interacting particles every timestep (fs)

1. Forces on particles f_i determined from the gradient of the interaction potential energy V

2. Acceleration vectors r_i calculated by integrating EoM

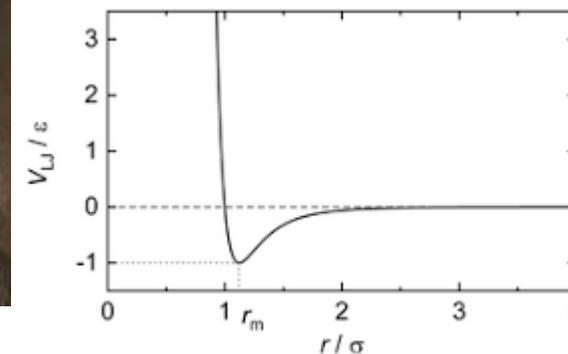
3. Forces and accelerations used to determine new positions and velocities

- Process repeated over many timesteps
- Utilise periodic boundary conditions to simulate a larger system

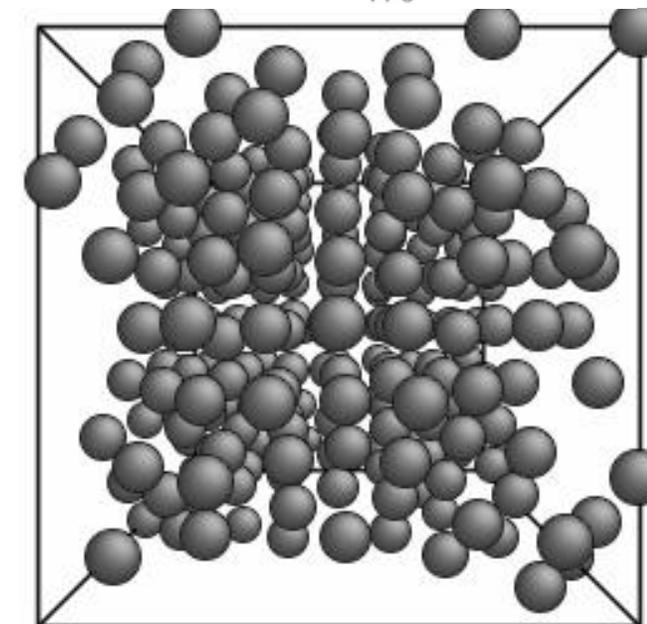
$$F = ma$$

$$f_i = -\nabla_{r_i} V$$

$$\ddot{r}_i = f_i / m_i$$



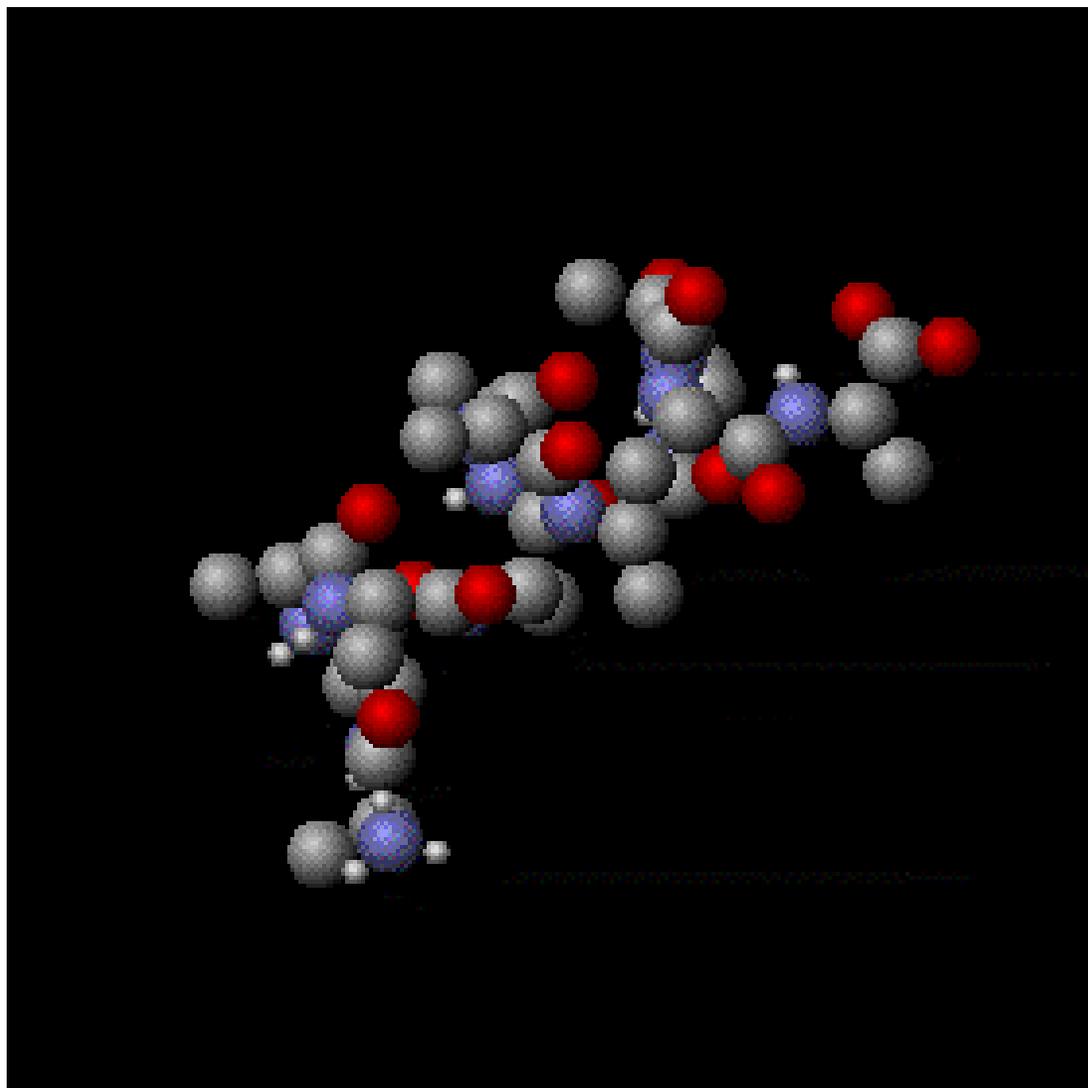
Alder and Wainwright. *J. Chem. Phys.* **27**, 1208 (1957)

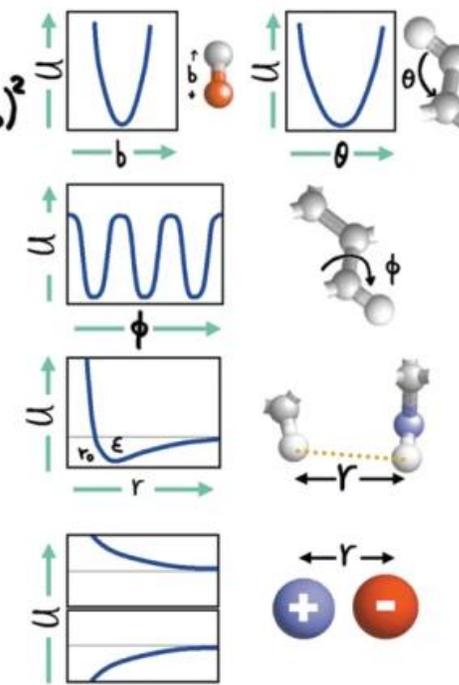


MD simulation of liquid argon

Rahman. *Phys. Rev.* **136**, A405 (1964)

Molecular Dynamics



$$\begin{aligned}
 U = & \sum_{\text{All Bonds}} \frac{1}{2} K_b (b - b_0)^2 + \sum_{\text{All Angles}} \frac{1}{2} K_\theta (\theta - \theta_0)^2 \\
 & + \sum_{\text{All Torsion Angles}} K_\phi [1 - \cos(n\phi + \delta)] \\
 & + \sum_{\text{All nonbonded pairs}} \epsilon \left[\left(\frac{r_0}{r} \right)^{12} - 2 \left(\frac{r_0}{r} \right)^6 \right] \\
 & + \sum_{\text{All partial charges}} \frac{332 q_i q_j}{r}
 \end{aligned}$$


Levitt. *Nat. Struct. Biol.* **8**, 392-393 (2001)

Nobelpriset 2013 The Nobel

The Nobel Prize in Chemistry 2013



Martin Karplus
Université de Strasbourg,
France and Harvard
University, Cambridge,
MA, USA

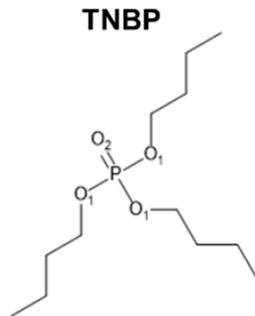


Michael Levitt
Stanford University School of
Medicine, CA, USA

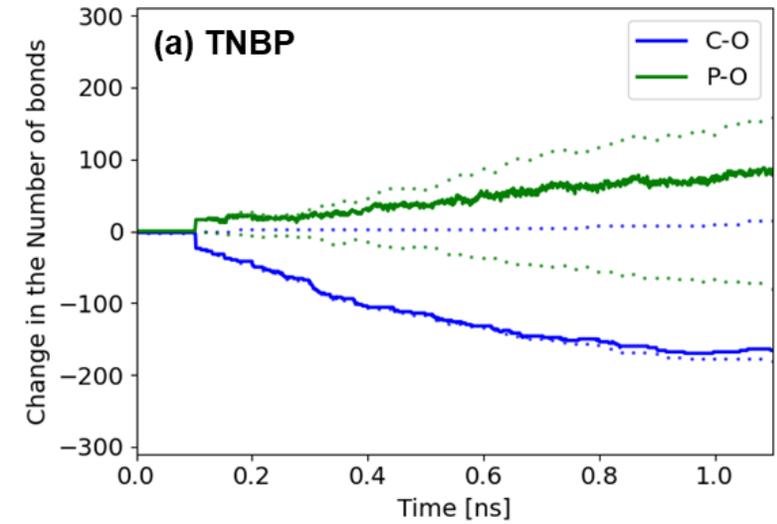
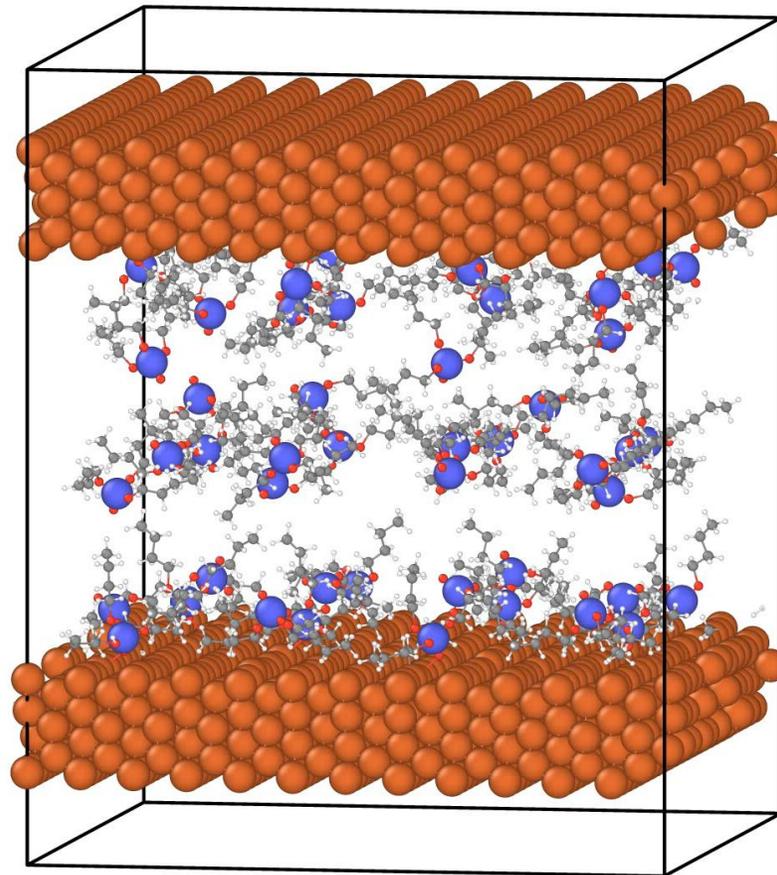


Arieh Warshel
University of Southern
California, Los Angeles, CA,
USA

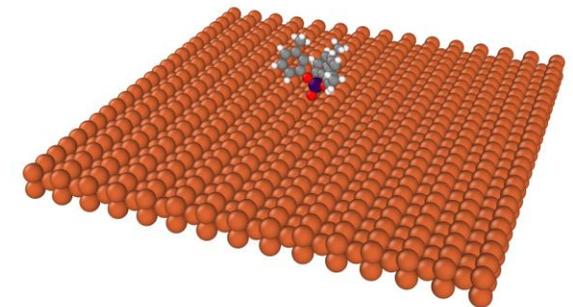
Lubricant Additives



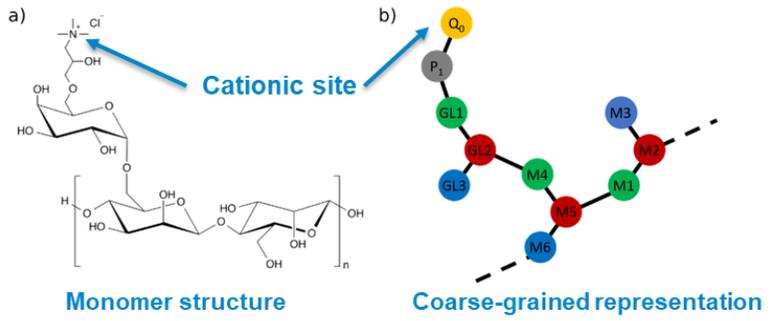
Non-Equilibrium Molecular Dynamics (NEMD)



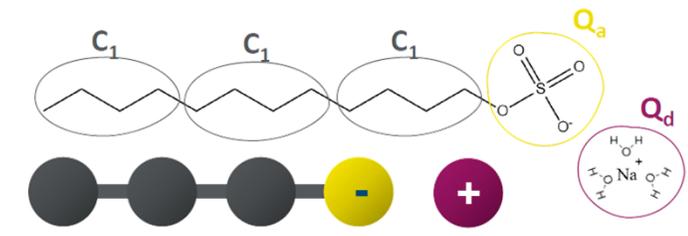
Kinetic Monte Carlo/MD (KMC/MD)



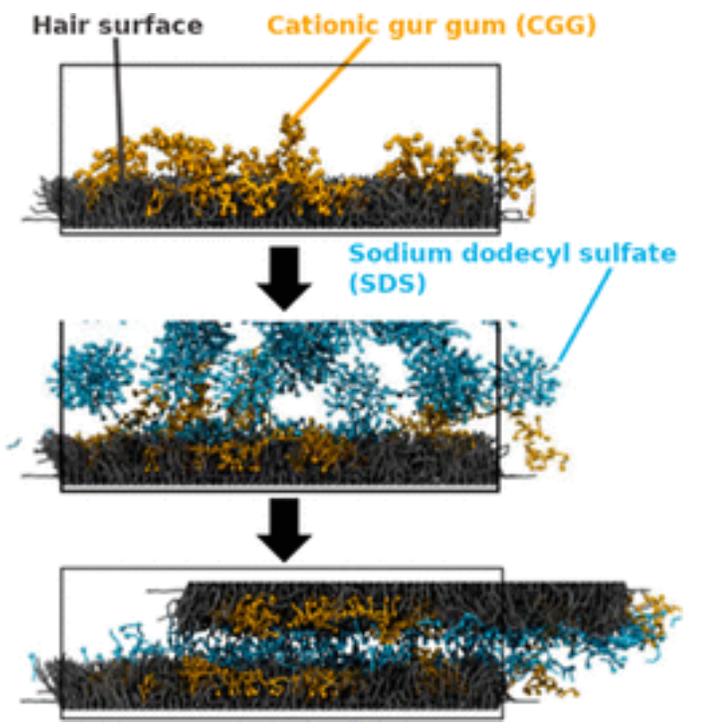
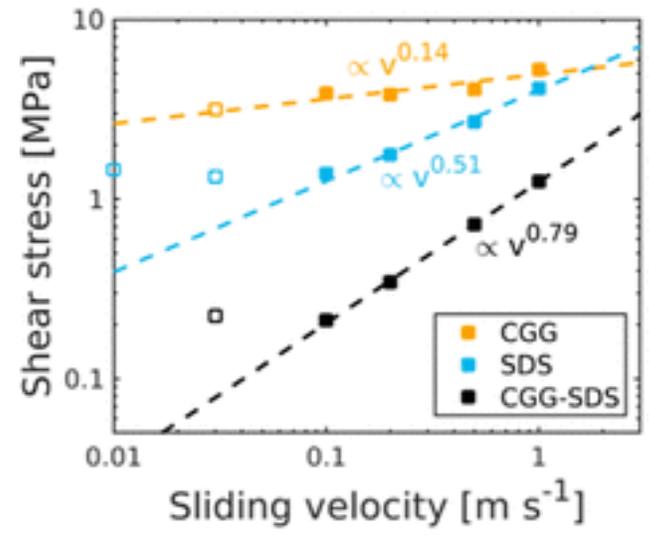
Conditioning: Cationic guar gum (guar hydroxypropyltrimonium chloride)



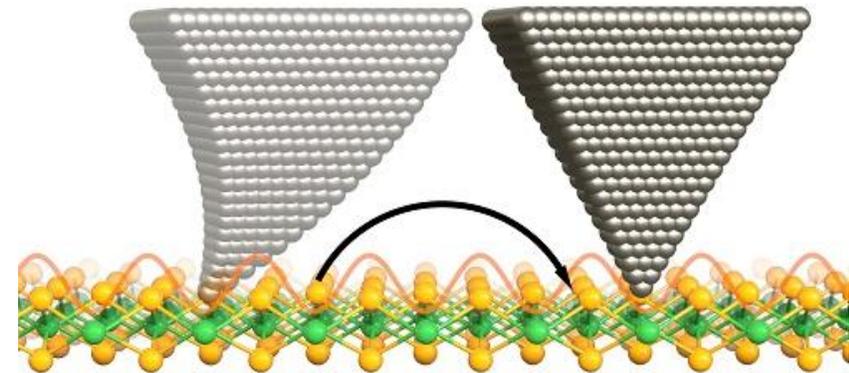
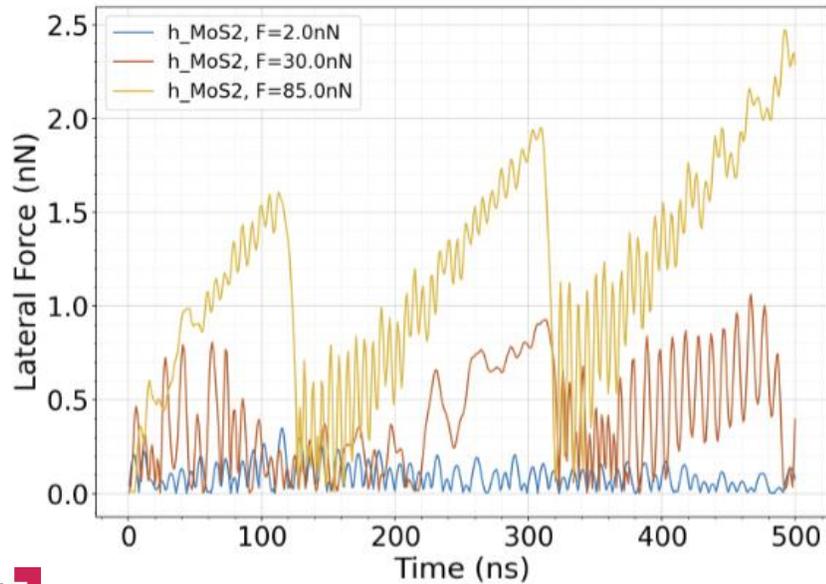
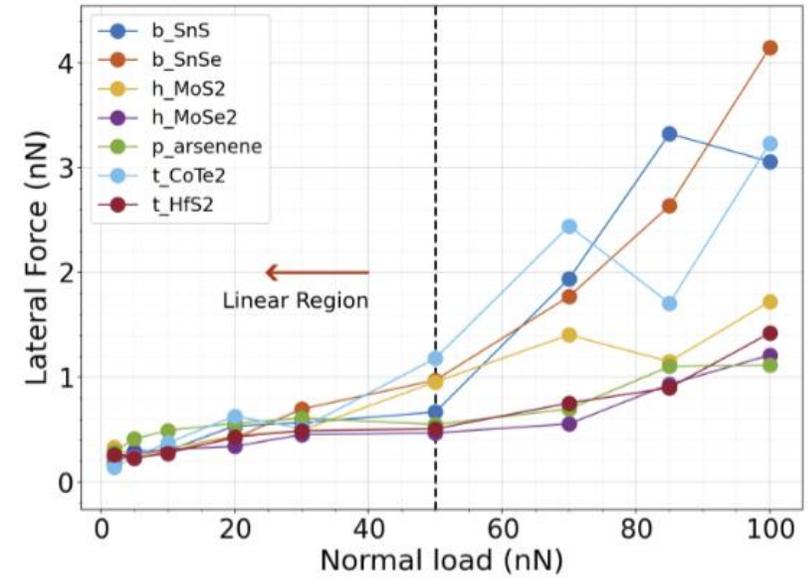
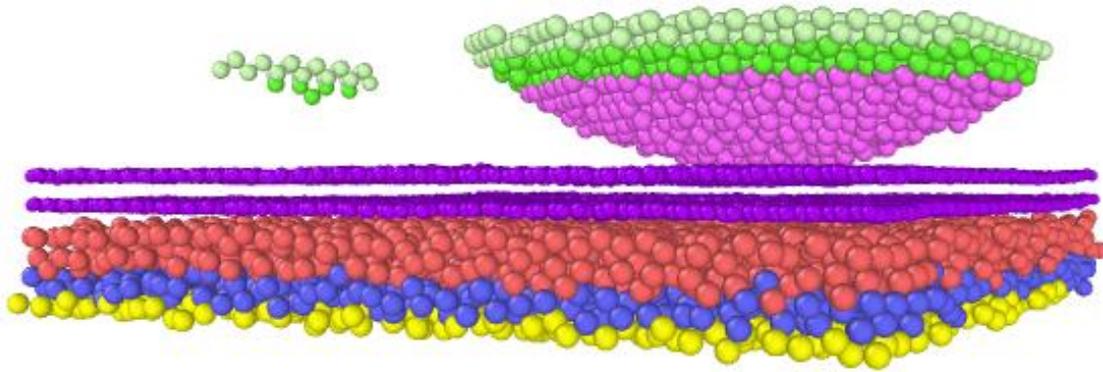
Cleansing: Sodium dodecyl sulfate (SDS)



Synergistic friction performance between CGG and SDS



Solid Lubricants



Song et al. *Phys. Rev. Lett.* **133**, 136201 (2024)

Acknowledgements

IMPERIAL

