

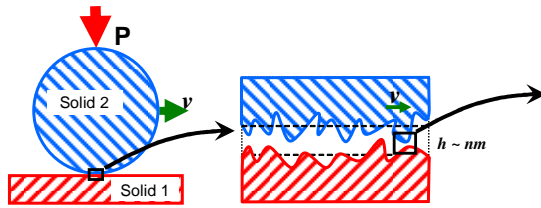
# Molecular Dynamics simulation of ZDDP effects on friction in nano-scale lubricated contacts

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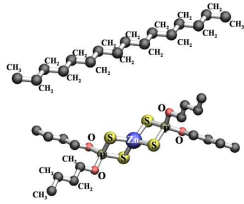


## Modelling lubrication at the nanoscale

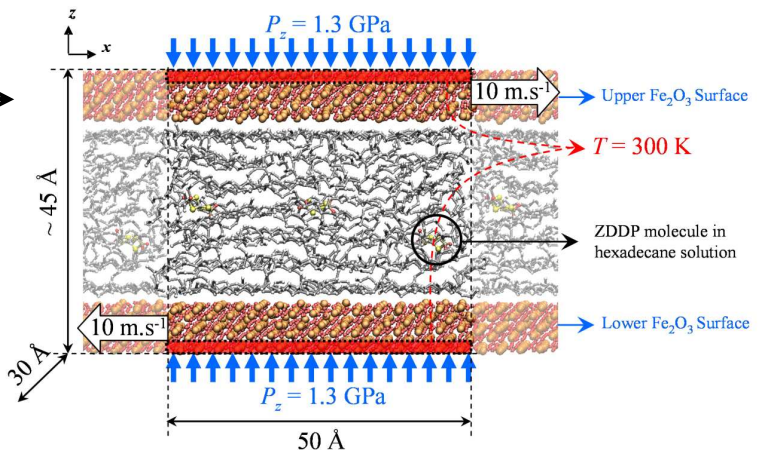
### A multiscale framework for lubrication modelling



Lubricant : mixture of n-hexadecane and ZDDP



- United Atom (CH<sub>2</sub> and CH<sub>3</sub> groups are considered as one interaction site)
- OPLS force field: considering inter and intramolecular interactions
- Intermolecular interactions: Lennard-Jones and Coulomb



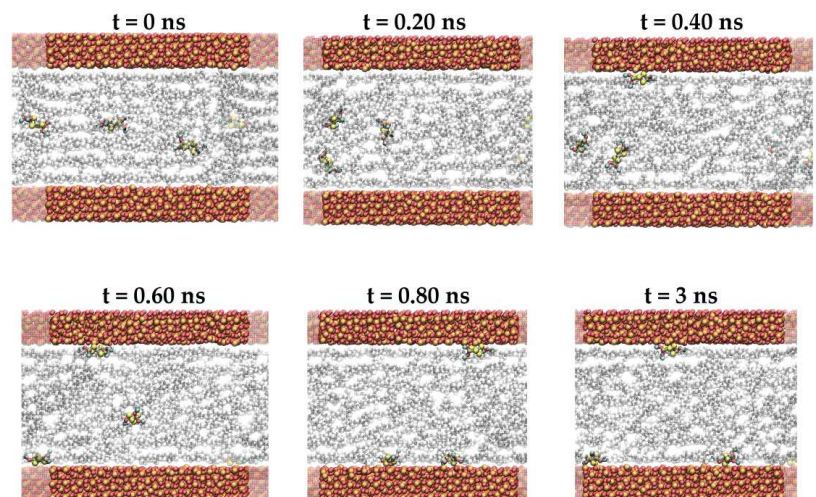
## The story

**Molecular Dynamics simulations** are used to study the tribological performance of a lubricant mixture containing hexadecane base oil and 5% Zinc Dithiophosphate (ZDDP) under molecular confinement conditions. The influence of ZDDP additive on the interfacial response is studied in detail. Simulations demonstrate the **migration of ZDDP** molecules and their **adsorption** onto the solid surface resulting in a remarkable **suppression of wall slip** compared to pure hexadecane. Consequently, the effective shear rate is higher and so is **friction**.

## Reference

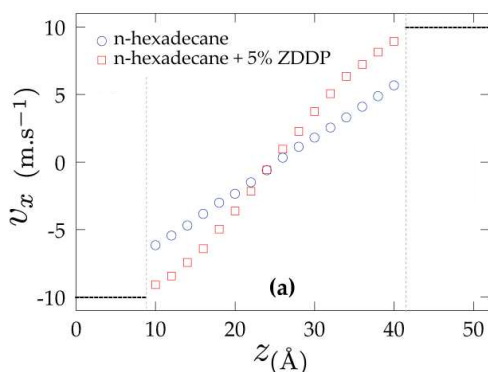
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## ZDDP migration and adhesion to the surfaces



Simulations carried out using LAMMPS [Sandia Laboratories] on P2CHPD facilities [FLCHP]

## Effect on wall slip and friction



- With ZDDP adsorbed on iron oxide surfaces, wall slip is greatly reduced.
- The effective shear rate  $\dot{\gamma}$  of the lubricant significantly increases.
- As a result, shear stress  $\tau_{xz}$ , representing friction, also increases.

Film composition	$\dot{\gamma}$ (x 10 <sup>9</sup> s <sup>-1</sup> )	$\tau_{xz}$ (MPa)
100% n-hexadecane	4.30	93.6
95% n-hexadecane+ 5% C4-ZDDP	8.26	115.7

This friction increase caused by ZDDP addition is in accordance with reported experimental findings.

MD simulations propose an explanation of this phenomena.

