WETTABILITY@Al_2O_3: ADSORPTION OF LUBRICANT ADDITIVES BY MOLECULAR MODELING

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ABSTRACT
In lubricant development, changes in formulations triggered by modifications of legislations, might affect the behavior of the lubricant towards the surface. This can lead to modifications of the wettability properties and the ability of the lubricant to spread over the surface. Better wettability involves a better adhesion of the lubricant on the surface and a faster wettability kinetic. Therefore, it is important to better understand the interactions between the lubricant and the surface, and how wettability can be linked to the lubricant formulation.

In this study, we use density functional theory calculations to describe the interactions at the interface between the lubricant and the surface.

Here, we focus on industrial lubricants for applications in metal working, especially on aluminum sheets. As aluminum oxidizes immediately when exposed to air, γ-Al_2O_3 has been chosen as a model for the surface. The major interaction of the lubricant with the surface comes from the additives it contains. For this reason, the solid-liquid interactions studied here are the ones between the surface and the functionalized head groups of the additives, which is equivalent to consider that their carbon chains are all the same. This study has been conducted on a wide range of head groups: polar molecules, apolar molecules, functionalized aromatics and phosphorous compounds.

By comparing the adsorption energies of different additives on the surface and their solvation energies in a model lubricant base oil, we aim at determining the influence of the different types of additives in the wetting process. Indeed, it has been shown that up to a certain point, solid-liquid interactions favor the wetting of the surface [1]. As a consequence, good additives should have the tendency to go to the solid-liquid interface rather than to stay in the liquid bulk. As the solvation energies obtained for the different head groups are quite similar (Fig. 1), they are not a significant parameter to discriminate the additives, contrary to the adsorption energies. Phosphates and carboxylic acid are the most adsorbed head groups (Fig. 1). For this reason, the additives containing these head groups should improve the lubricants wettability on aluminum sheets better than the ones containing head groups which are less adsorbed as water, alcohols and esters for example.

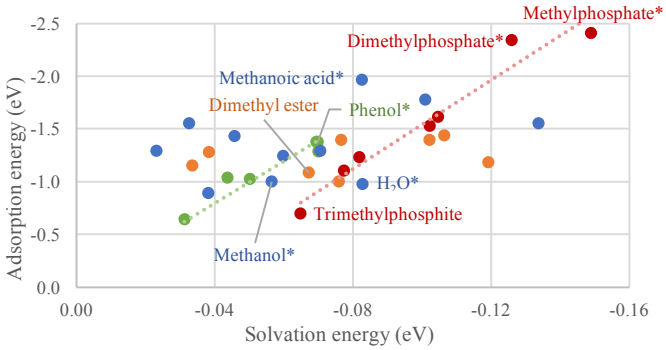

Fig. 1 Comparison of adsorption and solvation energies for various head groups: polar molecules (blue), apolar molecules (orange), functionalized aromatics (green) and phosphorous compounds (red). * indicates dissociative adsorptions.

In conclusion, the results obtained are consistent with previous studies, showing that acids are improving dynamic wetting of an oil on aluminum better than alcohols and esters [2] and that phosphates are better lubricant additives that phosphites, as the friction coefficient of an oil on aluminum can be reduced by adding phosphates whereas phosphites are increasing it [3].

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