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Adsorption of lubricant additives made simple: DockOnSurf package

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DockOnSurf is a program written in Python 3 for automatically finding the most stable geometry of adsorbates on top of a solid surface. The method has been tested with a set of different adsorbates covering the whole range of nonmetal elements and a variety of organic functional groups interacting over two different surfaces at two different hydration states namely, hydrated and dehydrated hematite (0001) and γ-alumina (100). DockOnSurf has interesting potential for *in silico* design of lubricants.

Keywords: Adsorption, Lubricant additives, Surface properties, Density Functional Theory

1. Introduction

Lubrication plays a major role in a wide range of industrial sectors such as energy and mobility. Changes in formulations triggered by modifications of legislations might affect the behavior of the lubricant towards the surface. This can lead to variation of the wettability or tribological properties among other factors. Computational chemistry based on density functional theory (DFT) was shown to be a powerful tool to describe interactions at the additive/surface interface. As additives are often large multifunctional molecules, it is hard to predict which function will adsorb on which site of the surface and trying all configurations by hand is long and fastidious. Therefore, an automated workflow DockOnSurf has been developed.

.Methods

The algorithm tackles the problem in a systematic manner by splitting the whole procedure in three consecutive stages: I) Selection of gas-phase conformers with promising structures to be adsorbed. II) Screening of the different conformer structures adsorbed on the surface in multiple orientations and adsorption sites with quick methods. Proton dissociation is also considered. III) Refinement of most stable step-II structures with accurate DFT calculations. All DFT calculations were performed with CP2K, using an hybrid gaussian and plane waves (GPW) method [1, 2].
The adsorption energy of a molecule on a given surface is defined as:

$$E_{ads} = E_{molecule@surface} - (E_{surface} + E_{molecule})$$

2. Results & Discussion

We have determined the influence of different types of additives in the surface properties modification: wetting process, adhesion, lubrification, passivation etc. The adsorption energies of different functional groups on both hematite and alumina are presented in figure 1. Hematite is more reactive towards different types of head groups than alumina. The results have shown that more acidic molecules tend to bind more strongly on the surface as they are more likely to be dissociated when adsorbed on both surfaces.

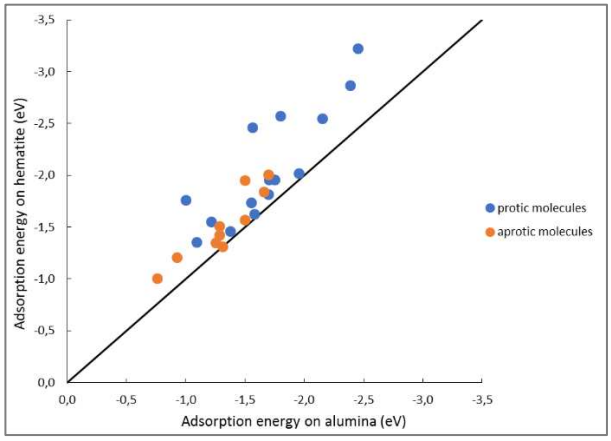

Figure 1: Comparison of adsorption energies obtained for different molecules on alumina and hematite surface [3].

This method enable to classify more complex molecules (figure 2) with its adsorption strength. This properties can be directly or indirectly linked to macroscopic performance and ca help for *in silico* design of new additives.

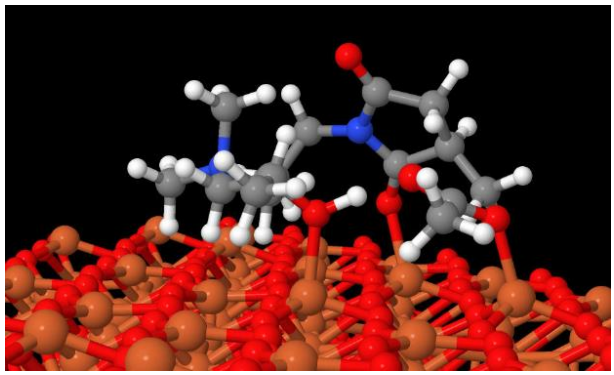

Figure 2: Optimized structure: adsorption multi-functional additives on iron oxide surface

3. References

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