Effects of iron oxide layers on adsorption mechanism of C18 fatty acid: A computational study

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1. Introduction

In the automotive industry, the control of friction and wear by the lubricant in thermal engines is one of the most important issues for fuel economy. Therefore, it is needed to better understand the nature of tribochemical reactions in order to design and develop better lubricants that also address environmental requirements. C18 fatty acids seem to be good candidates to achieve this target. In this study, we have investigated the adsorption mechanism of some organic friction modifiers on different iron-based surfaces.

2. Material and methods

The computational chemistry approach can give us dynamic information at the atomistic and electronic levels. An ultra-accelerated quantum chemical MD (UA-QCMD) simulator "Colors-Ryudo" has been developed in order to deal with chemical reaction dynamics for large complex systems [1]. We have applied these methods to study the adsorption mechanismof C18 (saturated and unsaturated) fatty acid e.g. stearic, oleic and linoleic acids which are organic friction modifiers on different iron based surfaces choose with respect to a steel surface study[2]: pure iron, iron oxide Fe_2O_3 and iron oxide FeOOH.

3. Results

In this work, different orientations of fatty acid will be studied on each iron based surfaces. Main results are gathered on Table 1. Molecule is always chemisorbed through the acid groupon pure iron.
If the position is imposed, molecule is physisorbed on FeOOH but free molecule doesn't interact with FeOOH.
Orientation of the molecule toward the Fe_2O_3 surface has an impact on the adsorption mechanism. Depending on the angle between the acid group and Fe_2O_3, molecule can be physisorbed as shown on figure 1 or chemisorbed through the acid group.

Table 1: Adsorption mechanism summary regarding the surface type for single molecule adsorption

Iron-based surfaces	Adsorption mechanism
Pure Iron	Chemisorption
Iron Oxide Fe_2O_3	Physisorption/Chemisorption
Iron Oxide FeOOH	No adsorption/Physisorption

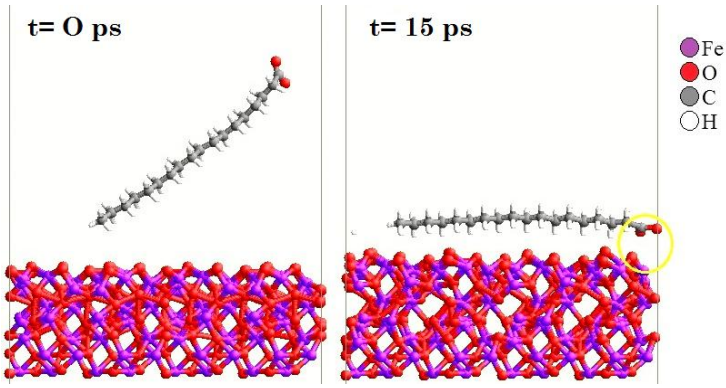

Figure 1:Adsorption of Stearic acid on iron oxide Fe_2O_3 surface at 50 °C studied bu UA-QCMD: initial step (left snapshot), final step (right snapshot)

4. Conclusion

The adsorption mechanism of C18 fatty acids on iron based surfaces has been successfully studied by UA-QCMD. The most the iron surface is oxidized; the less it is reactive with the fatty acid.

These results can be confirmed by experimental surface characterizations.

5. References

[1] Korshed A. et al. Cat. Today 164 (2011) 9–15
[2] Olla M et al. Surf.Int.Analysis, 38 (2006) 964-974