Theoretical Investigation of Carboxymethylcellulose/Glyceryl Monooleate Adsorption on Hematite

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INTRODUCTION

Understanding the behavior of polymer/surfactant mixtures at the interface is very important because of their widespread industrial applications such as painting, detergency, water treatment, and oil recovery.[1] Density functional theory was used to study the polysaccharide carboxymethylcellulose (CMC) [Fig.1], the surfactant glyceryl monooleate (GMO) [Fig.2], the CMC-GMO system, and their interaction with hematite. The results showed that CMC adsorbs preferentially on hematite and that the GMO interacts with CMC by hydrogen bonds and van der Waals forces. Based on these results molecular dynamics calculations were performed to better understand how polymer/surfactant interacts on the interface with hematite.

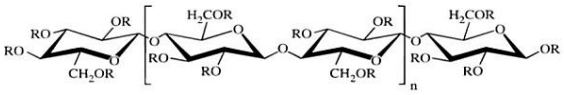

Figure 1. CMC.

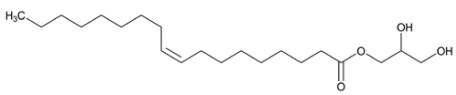

Figure 2. GMO.

METHODS

The interaction surface-polymer-surfactant was investigated with adiabatic molecular dynamics using the Dreiding II force field, trajectories of 1000ps with the CMC connected to the surface through the oxygen atom of the carboxymethyl group, and the (001) surface of hematite from the database of Cerius 2. The dynamics were performed in the presence or absence of surfactant, varying the size of the CMC fragments and their degree of substitution (DS). A preliminary study of the degree of surface coverage was also performed, considering two CMC fragments bounded to the hematite surface.

RESULTS AND DISCUSSION

The binding energy per fragment of CMC on hematite surface [Fig.3] ranges from 327.4 to 490.7 kcal/mol for dimers; 576.3 to 937.5 kcal/mol for tetramers; 914.3 to 1525.8 kcal/mol for octamers, becoming larger as the polymer chain increases. For the dimers the DS does not appear to affect the degree of interaction, however for the tetramers and the octamers an increase in the binding energy with increasing the DS is observed.

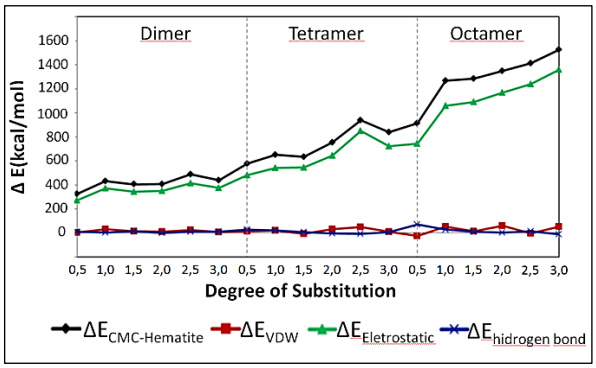

Figure 3. Binding Energy of CMC to Hematite.

The addition of the GMO increased the system stability in most cases by 100-200kcal/mol. The increase in binding energy of CMC to hematite in the presence of GMO can be explained by the reduction of the polymer intramolecular interactions such as hydrogen bonding.

CONCLUSIONS

The results indicate that CMC-hematite interaction is mainly governed by electrostatics forces. The molecular dynamics calculations showed that the addition of GMO increases the binding energy of CMC on hematite.

ACKNOWLEDGMENTS

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[1]Grządka, E., 2011.Materials Chemistry and Physics, 126(3), pp.488–493, (2011).