PhD Research Proposal Form
China Scholarship Council (CSC) - ENS Group

FIELD: CHEMISTRY

Thesis subject title: Atomistic simulations of surface coating in corrosive environment

Name of the French doctoral school : Ecole Doctorale de chimie

Name of the Research team : Theoretical Chemistry and molecular thermodynamics
Website : www.ens-lyon.fr/CHIMIE

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Lab Language : French and English

Research Proposal Abstract :

In the quest of sustainable innovative surface coatings, several challenges need to be addressed: (i) reduce the use of non-sustainable elements as P (ii) use aqueous formulations (iii) ensure high performance in adhesion and corrosion protection. To accelerate this quest, a greater understanding of the complexity governing adhesion is required. The impact of the chemical structure of the functional groups on adhesion performance and the resistance of the resulting composite materials to the environment are key points of interest of this PhD work. They will be investigated using atomistic modeling, benefiting from recent developments done in the Theoretical Chemistry group of the Laboratoire de Chimie of the ENS de Lyon.

The binding of various functional groups was investigated on both hydrated and dry alumina at the ab initio level, identifying carboxylates as promising binding groups.[1,2] We will focus on organic surface coating agents including only carboxylate groups. To start, we will investigate the binding of monomers and small oligomers containing a few carboxylic groups at the DFT level, assessing the binding sites and binding strength. Flexible and polyfunctional molecules will be easily adsorbed on the substrate with the open-source python package DockOnSurf[3] to obtain the optimized low-energy adsorption configurations. Our SolvHybrid scheme[4] will provide a routinely available semiquantitative determination of adsorption energies at the metal/water interface to provide a first assessment of the influence of an aqueous environment. Then, we will parametrize an interfacial force field to describe the carboxylate/alumina interaction using our GLJ approach.[5] This force field is built using a pair-wise approach and showed a high transferability. This will open the door to the exploration of the substrate hydration, effect of salt (Na^+, Cl^-), pH, and the presence of

multivalent metals, e.g. Al^{3+} and thus provide a deep understanding of the impact of the environment (air, water, salts) on the adhesion.

References :

[1] S. Blanck, S. Loehlé, S. N. Steinmann, C. Michel, *Tribology International* **2020**, *145*, 106140
[2] S. Blanck, C. Martí, S. Loehlé, S. N. Steinmann, C. Michel, *The Journal of Chemical Physics* **2021**, *154*, 084701
[3] C. Martí, S. Blanck, R. Staub, S. Loehlé, C. Michel, S. N. Steinmann, *Journal of Chemical Information and Modeling* **2021**, *61*, 3386-3396
[4] P. Clabaut, B. Schweitzer, A. W. Gotz, C. Michel, S. N. Steinmann, *J Chem Theory Comput* **2020**, *16*, 6539-6549.
[5] J. Rey, S. Blanck, P. Clabaut, S. Loehlé, S. N. Steinmann, and C. Michel, The Journal of Physical Chemistry B 125, 10843 (2021); X. Wu, S. N. Steinmann, C. Michel, *ChemRxiv* **2023**.

Type of PhD :

1.Full PhD

- Joint PhD/cotutelle (leading to a double diploma) : NO
- Regular PhD (leading to a single French diploma) : YES

2. Visiting PhD (for students enrolled at a Chinese institution who will be invited to a French institution to carry out a mobility period) : NO