New “green” corrosion inhibitors:

Theoretical study of corrosion inhibition of aluminum and Al-Cu alloys

Laboratory

CIRIMAT - Centre Interuniversitaire de Recherche et Ingénierie des Matériaux

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Advisor

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The proposed work focuses on fundamental surface physico-chemical processes. The scientific approach of the project is oriented towards applied innovation with industrial purposes. The studied materials (aluminum and later aluminum alloys) are widely used in aeronautics for instance and corrosion of metallic surfaces has a huge economic and environmental adverse impact with estimated costs of worldwide corrosion damage of about 2 billions EUR per year. Any improvement of corrosion protection has therefore large economic benefit.

In certain environments, such as in presence of Cl ions, aluminum and alloys become highly susceptible to localized corrosion. The use of corrosion inhibitors is one of the most effective and practical methods of corrosion protection and new standards, i.e. the “REACh” (Registration, Evaluation, Authorization and Restriction of Chemicals) European regulations push forward fundamental research to propose new green corrosion inhibitors. This PhD subject falls into this ambition.

Because of the complexity of corrosion and its inhibition processes, effective inhibitors are mainly determined in an empirical manner out of large sets of compounds, where experimental testing provided the information of whether a specific molecule is effective or not for a certain substrate in a given medium. We seek for a rational design of new inhibitors to provide a major breakthrough in the field of corrosion protection. To that aim we want to study several organic molecules that could be used as corrosion inhibitors. We will consider the molecules-surface interactions in relation to corrosion inhibition. Some pioneers works were already presented in the literature (Costa *et al.*[1] , Kokajl and al.[2], Chiter and al.[3,4]) but new fundamental understanding of the elementary events leading to corrosion and corrosion inhibition is still required.

First, calculations will be done on realistic atomistic model oxides starting from experimental data, to study elementary events of corrosion initiation by chlorides within the Density Functional Theory (DFT) framework (adsorption, insertion, diffusion, bond breaking). Several chloride concentrations and Al extraction/dissolution will be taken into account.

Secondly, DFT calculations will be carried out in the presence of potential inhibitors (silanes, phosphonates, amines or carboxylates). We will model self-assembling of corrosion inhibitors on surfaces with a focus on the efficiency of the surface functionalization on the inhibition

ability. The presence of an inhibiting layer will be introduced by considering DFT-based energetics to propose new solutions for corrosion inhibition on realistic systems.

Collaborations

At CIRIMAT, the collaboration with Nadine Pébère, expert in electrochemical techniques (global and local) used to assess the efficiency of corrosion inhibitors, will help in the choice of the models and the validation of computational results.

Morever the PhD student will benefit from the collaboration between Corinne Lacaze-Dufaure and D. Costa (ENSCP, "Physico-Chimie des Surfaces" laboratory).

Candidate profile

Candidates with background in chemistry, physics, chemical-Physics. Master courses in theory and simulations will be welcome.

Applications

Please send an email to Prof Corinne Lacaze-Dufaure, including a detailed CV, letter of motivation, and copies of marks for Master years and before. Supporting letters will also be necessary afterwards.

Deadline for application is 7th April 2017, for starting date 1st Oct 2017.

[1] Molecular Modeling of Corrosion Processes: Scientific Development and Engineering Applications, D. Costa and P. Marcus (eds C. D. Taylor and P. Marcus), John Wiley & Sons, Inc, Hoboken, NJ. doi: 10.1002/9781119057666.ch5 (2015)

[2] What determines the inhibition effectiveness of ATA, BTAH and BTAOH corrosion inhibitors on Copper?, A. Kokalj, S. Peljhan, M. Finsgar, I. Milosev, JACS, 132, 16657 (2010).

[3] DFT Studies of the Bonding Mechanism of 8-Hydroxyquinoline and Derivatives on the (111) Aluminum Surface, F. Chiter, C. Lacaze-Dufaure, H. Tang, N. Pébère, Physical Chemistry Chemical Physics 17, 22243 (2015)

[4] Fatah Chiter, PhD thesis, Institut National Polytechnique de Toulouse, Novembre 2015.