

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM (one page maximum)

Field: Chemistry, Physical Chemistry and Chemical Engineering

Subfield: Surface Science, Molecular Modeling

Title: Organic molecules for the corrosion inhibition of Al alloys: theoretical and experimental model approach

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: Dominique COSTA (Dimitri Mercier, Sandrine Zanna, Philippe Marcus co-advisors)

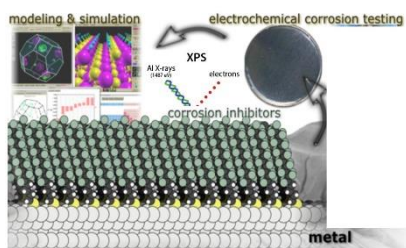
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Research group/Lab: PSC/IRCP

Lab location: 11 rue P et M Curie 75005 Paris

(Lab/Advisor website): <https://www.ircp.cnrs.fr/en/la-recherche/equipe-pcs/pcs-group/>

Short description of possible research topics for a PhD:



The corrosion of metals is a universal phenomenon with significant economic and societal impacts and their protection has become a major issue. This thesis subject aims to target new organic coatings allowing an improvement in the corrosion resistance of Al alloys as well as a reduction of the environmental load compared to existing coatings. We propose to develop a rationalized search for organic inhibitors based on a combined theoretical / experimental approach aimed at understanding i) molecule / surface interactions at the atomic scale, ii) the 2D and 3D self-organization in dense layers of organic molecules on metal surfaces and iii) the corrosion resistance of the metal surfaces thus

functionalized. This approach, coupling modeling by DFT, advanced characterization of surfaces (XPS, ToF-SIMS, AFM) and electrochemical measurements will be applied to Al alloys and to specific organic anchoring molecules (silanes, phosphonates), which are known to be effective in Al corrosion inhibition.

Required background of the student:

The applicant should have a solid physico-chemical (material sciences) background together with a formation in theoretical chemistry.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Cornette, P.; Zanna, S.; Seyeux, A.; Costa, D.; Marcus, P. The Native Oxide Film on a Model Aluminium-Copper Alloy Studied by XPS and ToF-SIMS. *Corros. Sci.* **2020**, *174*, 108837
2. Poberžnik, M.; Chiter, F.; Milošev, I.; Marcus, P.; Costa, D.; Kokalj, A. DFT Study of N-Alkyl Carboxylic Acids on Oxidized Aluminum Surfaces: From Standalone Molecules to Self-Assembled-Monolayers. *Appl. Surf. Sci.* **2020**, *525*, 146156.
3. Vernack, E.; Costa, D.; Tingaut, P.; Marcus, P. DFT Studies of 2-Mercaptobenzothiazole and 2-Mercaptobenzimidazole as Corrosion Inhibitors for Copper. *Corros. Sci.* **2020**, *174*, 108840.
4. I. Milošev, T. Bakarič, S. Zanna, A. Seyeux, P. Rodič, M. Poberžnik, F. Chiter, P. Cornette, D. Costa, A. Kokalj, P. Marcus - Electrochemical, Surface-Analytical, and Computational DFT Study of Alkaline Etched Aluminum Modified by Carboxylic Acids for Corrosion Protection and Hydrophobicity – J. Electrochem. Soc., **2019**, 166 (11), C3131-C3146.
5. A Kokalj, D. Costa, Molecular Modeling of Corrosion Inhibitors **2018** Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry Chapter: 13444, 332-345, Elsevier Inc.