Research Grants for PhD students from the China Scholarship Council

Information Form (please read the guidelines carefully on the website www-csc.utt.fr)

Supervisor's name : Huang | Given names : Xian

Status (prof., assistant prof., …) : Associate professor (maître de conférences)

Laboratory :	MATEIS	Website address :	https://mateis.insa-lyon.fr/en
Institution :	INSA Lyon	Website address :	https://www.insa-lyon.fr/en/

Scientific competence of the supervisor:

1. corrosion phenomenon modeling (passive film growth, defect chemistry and diffusion in oxides, alloy substrate degradation);
2. atomic scale simulations (DFT, MD);
3. materials characterizations and analyses (electrochemistry, electronic microscopy, etc.)

Two major publications in the field proposed for the PhD :

1. X. Huang, D. Costa, V. Maurice, P. Marcus, Applied Surface Science 716 (2026) 164709.
2. D. Chen, C. Dong, G.R. Engelhardt, J. Qiu, D.D. Macdonald, Corros. Sci. 248 (2025) 112779.

Website address of the personal page : https://www.researchgate.net/profile/Xian-Huang-12?ev=hdr_xprf

Supervisor's email : xian.huang@insa-lyon.fr

Description of the research work proposed for a PhD ***Topic # (see list) :*** IV-6

Title : Atomic scale modeling of passive film growth

Subject :

Passive films formed on electrically polarized alloy surfaces can enhance corrosion resistance but also, in some cases, deteriorate surface functionality for electrochemical applications. Modeling passive-film growth and predicting film properties are therefore essential for the optimizing material durability and performance. The Point Defect Model (PDM), developed to describe growth kinetics by considering defect-related reactions and diffusion, has been successfully applied to qualitatively explain various electrochemical observations. However, quantitatively predicting electrochemical behavior remains challenging due to the lack of experimental data on defect-related properties for most oxides and hydroxides.

To adress this issue, this research project proposes to investigate the defect-related reactions and diffusion using Density Functional Theory (DFT), combined with the Transition State Theory (TST). This ab initio approach not only can provide atomic-scale insights into defect behavior in passive films, but also enables the computation of thermodynamic, thermokinetic and electronic parameters required by the PDM, with minimal empirical input. For validation, the computational results can be compared with experimental electrochemical measurements, including Electrochemical Impedance Spectroscopy (EIS), performed in the MATEIS laboratory.

Keywords :

passive film, electrochemistry, DFT, EIS

Expected collaborations :

The position will be based in the MATEIS laboratory.

DFT calculations will be carried out using the remote computing resources of the regional and national high-performance computer centers, under the supervision of Dr. X. Huang (MCF). Electrochemical analyses will be under the supervision of Dr. S. Marcelin (IR, HDR) and Pr. B. Normand (PR, HDR).

Background required from the applicant :

Highly motivated students with a master's degree in materials science and engineering, or an equivalent field, are strongly encouraged to apply. Experience in electrochemical analysis, passive film modeling or DFT calculations will be considered an advantage.

Existence of a PDF file detailing the proposal ("yes" or "no") : no

(see guidelines on the website www-csc.utt.fr)