Pit propagation and complex structures formation during the degradation of 2D iron nanofilms

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Applications of 2D ultrathin oxide/metallic nanolayers extend over many different fields, from solar energy conversion, renewable energy, photocatalysis, electrocatalysis, electronics and protective coatings. Understanding their stability or their degradation (especially for non noble metal) is of particular importance in all these applications. In our case, we have recently worked on iron 2D nanofilms to explore first instants of the biocorrosion process, when bacteria suspended in liquid are in contact with the interfacial nanolayers [1]. To go further, a better characterization of the nanofilm degradation in aqueous medium without bacteria is needed. As shown by preliminary experiments, performed on droplets, pits, due to initial defects, propagate in 2D and create interesting and complexes structures (sunny-shape and self-similar structures).

The intern will work on the structures formation using both experimental and theoretical approaches. He/she will participate to a collaborative work, in which different researchers will bring their own expertise, offering the student a great opportunity to discover and learn about complementary approaches. On the one hand, nanofilm preparation and simple optical experiments will be done; additional experiments using bacteria might be planned at the end. On the other hand, theoretical approaches will be done with Mathis Plapp [2]. Multi-scale molecular modeling approach combining atomistic-scale density functional theory calculations [3] and molecular dynamics simulations as well as larger-microscopic-scale kinetic Monte Carlo simulations [4]) will be also transferred to the current project by Yun Hee Jang and Yves Lansac (visitors in the team).

No previous experience on the different domains is needed; we are just looking for motivated, sociable and curious candidates who are interested by a multidisciplinary project, involving theory, simulations and experiments.

[1] M. L..Herbette, C. Regeard, C. Marlière, et al. Biocorrosion on Nanofilms Induces Rapid Bacterial Motions via Iron Dissolution, ACS Central Science 7, 2021.

[2] K. M. Kolwankar, M. Plapp and B. Sapoval, Percolation-Dependent Reaction Time in the Etching of Disordered Solids, *Euro Physics Letters*, 62**,** 519, 2003.

[3] For example, A. Groß and S. Sakong, Ab Initio Simulations of Water/Metal Interfaces, Chemical Reviews 2022, 122 (12), 10746-10776

[4] For example, N. Snir and M. C. Toroker, Simulations to Cover the Waterfront for Iron Oxide Catalysis, ChemPhysChem, 23, e202200025, 2022.