Post-doc : *Ab initio* investigation of routes for improvement of adhesion zinc/alumina interface.

Employer : Institut des NanoSciences de Paris (INSP) - UMR 7588, CNRS & UPMC
Duration : 12 months

The Institute is a research unit associating the CNRS (National Center of Scientific Research) and Pierre and Marie Curie University (UPMC). Within the Institute, the team « Oxides in Low Dimensions » brings together experimentalists and theoreticians with a goal to explore the structure of oxide surfaces, thin films, and metal/oxide interfaces, and to understand their electronic, magnetic, adhesion, and reactivity properties.
More information : http://www.insp.upmc.fr/-Oxydes-en-basses-dimensions-.html
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Within the ongoing collaboration between Institut des NanoSciences de Paris (INSP) and the research and development center of ArcelorMittal the present project aims to explore routes for improvement of adhesion at zinc/alumina interface.
In fact, the adhesion at zinc/alumina interface is a key issue in the field of steel-making industry, where galvanization is a common method to protect steel against corrosion. Nowadays new steel grades known as high strength steels are purposely enriched in strengthening elements, such as Al, so that thinner steel sheets can be used, leading to a reduction of product weight and cost. However, the annealing of steel after cold rolling, results in a selective oxidation of Al and in surface segregation of alumina particles or films which are only poorly wetted by zinc, reducing dramatically the quality of the anti-corrosive Zn protection.
With a help of an *ab initio* calculations, the goal of the study is to identify the most weakly adhering zones at model Zn/alumina interfaces and to quantify the effect of: (i) interface doping, (ii) formation of interface oxides, and (iii) interface charge excess, to the Zn/alumina adhesion characteristics.

Applicants should hold a PhD degree, with a strong background in physics, theoretical chemistry, and/or computer science, oriented preferably towards oxide surfaces and interfaces. The candidate is expected to have a good experience in ab initio calculations, especially in what concerns an efficient construction and optimization of superstructures. Expected to interact with both ArcelorMittal engineers and University researchers, the ability to efficiently prepare scientific documents (reports, publications) and presentations in English is essential.