Ab initio study of adhesion improvement at zinc/silica interfaces.

Employer: Institut des NanoSciences de Paris (INSP) - UMR 7588, CNRS & UPMC
Duration: 12 months with a possibility of an extension
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Adhesion at zinc/oxide interfaces has become of key importance for steel-making industry where galvanic zinc remains the most common anti-corrosive protection. Indeed, since most modern steel grades are purposely enriched in strengthening elements (e.g., Si, Al, or Mn), their selective oxidation followed by oxide segregation to steel surfaces reduces dramatically the adherence of the Zn over-layer.

Within an ongoing collaboration between INSP and ArcelorMittal Maizières Research, the present project aims at exploring new routes for the improvement of adhesion at zinc/silica interfaces. The principal goal is to quantify the improvement of adhesion when using multicomponent buffers at the interface, based on interface energetics (adhesion and interface energies) of individual metal/metal, oxide/oxide, and metal/oxide interfaces, estimated at an ab initio (DFT) level, and on a thermodynamic Monte-Carlo model of buffer composition and structure under different oxidation conditions.

Applicants should hold a PhD degree, with a strong background in computational physics and/or chemistry, preferably oriented towards oxide surfaces and metal/oxide interfaces. The candidate is expected to have a good experience in (ab initio) atomistic calculations, 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.

The « Oxides in Low Dimensions » group at INSP 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