Internship offered in M2
2018-2019

Responsible for internship

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Group:

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Internship topic: Design of new metal/oxide thin films via ab initio modeling

The internship is at the crossing point between physics and nano-engineering, with potential consequences on both academic and industrial researches; it will be carried out within a collaboration between the INSP and Saint-Gobain Research Paris, an industrial research and development center of the Saint-Gobain group. Its main research areas are related to glass, thin films and surface coatings, aiming at elaborating new and innovative products that help reducing energy consumption and improve the well-being of people worldwide.

In this context, low-emissivity glazings based on thin-films technology are being developed for applications in the building and automotive sectors, in order to optimize thermal insulation. These coatings are made of nanometric stackings of different materials; in particular, infrared-reflecting metals such as silver are deposited by magnetron sputtering (or plasma vapor) techniques on metal oxide layers -- typically, zinc oxide. The macroscopic properties of those coatings, such as their mechanical durability or electronic conductivity, ultimately depend on atomiclevel interactions at the interface between the layers. Hence, a thorough understanding of these interfaces is crucial in order to design better coatings, which could be achieved via ab initio simulations.

This internship aims at modeling the structure and stability of the ZnO/Ag interface, and in particular at understanding the role of dopants, through ab initio calculations. For instance, Aluminum is frequently used as a dopant for the ZnO layers but its exact influence on the mechanisms driving the interface adhesion is not well known, as the experimental determination of its atomic structure and related properties is a formidable task. Additionally, in order to enhance the adhesion between the metal and the oxide, other metallic elements, such as NiCr or Ti, can be inserted at the interface. Their impact on the interface properties is crucial to the macroscopic properties of the whole glazing, especially its mechanical durability and performances. The study could be extended to designing optimal interfaces by analyzing those more complex configurations. The simulations, which will mainly rely on the DFT, will explore several distinct interfaces, as well as their corresponding mechanical and electronic properties, improving recent works.

Techniques involved: Ab initio (Density Functional Theory) calculations

Type of internship: theorical
Paid internship: Yes
Can this internship be continued for a PhD? Yes
If yes, type of PhD funding envisaged is: Bourse école doctorale ou CIFRE