

Séminaire - Anna Ferrari

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Séminaire

Pôle CAPT #Chimie Analytique, Physique et Théorique

[ex-Thème 1 - "Développements de concepts et méthodes de recherche"]

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In the last years, ZnS and ZnS derived materials have attracted an increasing interest as a possible green alternative to the currently used CdS photocatalysts for hydrogen production from water splitting via photothermochemical cycles. However, unlike CdS, ZnS does not naturally present a suitable band gap for photocatalytic applications (3.82 eV). Therefore the pristine material has to be engineered in the attempt to tune its band structure into the desired properties.

Despite the attracting potential applications of these materials, they have been the object of only a handful of works and a strategy for a successful band structure engineering has not yet identified. In addition the morphology, stability and reactivity of ZnS surfaces are still obscure.

In our work, density functional theory (DFT) periodic calculations have been employed in order to: i) exploit the extent of the band structure modulation achievable by means of a doping strategy with metal atoms (M). Among the possible metallic agents five transition metals (Ni, Co, Mn, Cu and Ag) and a III A group element (In) have been selected.; ii) ZnS surface characterization. The most stable surfaces have been identified and their reactivity has been investigated by probing the acidity and basicity of the ZnS surface sites with small molecules (H₂O, CO₂, CO, NH₃ and CHF₃), Figure 1; iii) understand the effects of nanostructuring on the electron properties of ZnS and ZnS derived materials.

Computed results have been compared with absorption (UV and IR) spectroscopy data recorded on particles synthesized in our laboratory.