Unraveling the semiconductors properties

Amanda F. Gouveia^{1,3*} (PG)*, Laécio S. Cavalcante¹ (PQ), Juan Andrés² (PQ), Elson Longo³ (PQ), *amanda@liec.ufscar.br

¹DQ-GERATEC, Universidade Estadual do Piauí, P.O. Box 381, 64002-150 Teresina, Piauí, Brazil

²Department of Analytical and Physical Chemistry, University Jaume I, 12071 Castelló, Spain

³CDMF, Universidade Federal de São Carlos, P.O. Box 676, 13565-905 São Carlos, São Paulo, Brazil

Keywords: surfaces, morphology, electron beam, nanoparticles.

It is known that the morphology, dimensionality and crystalline structure of materials play important roles in electronic, optical, catalytic properties, among others. Understanding the role of these surfaces and find a relationship with their physical and chemical are of extreme importance. The theoretical calculations of the surfaces provide a deep knowledge about the kind of superficial defect, i.e. oxygen vacancies and local distortions, and how they are linked with the semiconductor properties, such as decrease of the band gap value, improve in the photocatalysis among others.

On the other hand, advances in electron-matter studies, based on the irradiation of the electron beam in the transmission electron microscopy or field emission-scanning electron microscope on materials represents a preferred external physical and chemical tool for *in situ* remote command of the functional attributes of nanomaterials associated to its unique advantages of high spatial and temporal resolution and digital controllability. This makes the field of electron beam irradiation an emerging topic open for many researchers right now.

The formation of Ag nanoparticles is currently a topic subject to a great deal of research because they are excellent materials with many technological applications. Recently, the formation of Ag nanoparticles on α -Ag₂WO₄ semiconductors induced by electron irradiation has been reported.

A theoretical framework is developed to determine the physical principles involved in the mechanism for the formation of metal nanoparticles on different materials by electron beam irradiation under the guidance of first-principles calculations at density functional level.

The aim of this research is predict the morphology of semiconductors based on the Wulff construction and to describe the mechanisms of electron beam irradiation on α -Ag₂WO₄ and its transformation to form Ag nanoparticles in vacuum conditions. To this end, a combined study involving experiments and first-principles calculations is presented. With the increasing interplay between experimental and computational approaches at multiple length scales, it will be also discuss how these combined data can be used to provide a deep insight into the rationalization of electron beam-induced transformations.

Acknowledgments

The authors acknowledge the financial support of the Brazilian research financing institutions: CNPq (150949/2018-9; 312318/2017-0; 479644/2012-8, 304531/2013-8, 304531/2013-8), FAPESP (2013/07296-2), CAPES and Generalitat Valenciana.