BENEMÉRITA UNIVERSIDAD AUTÓNOMA DE PUEBLA

INSTITUTO DE FÍSICA
"Luis Rivera Terrazas"

SEMINARIO EXTRAORDINARIO
"DR. JESUS REYES CORONA"

"New Generation of Materials for More Efficient Solar Energy Use: Quantum Modeling and Experimental Realizations"

Prof. Dra. Perla Wahnón
Universidad Politécnica de Madrid

The intermediate band (IB) concept has been recently introdced to propose novel photovoltaic solar cell with enhanced efficiency1. To realize this principle we have proposed in recent years, on the basis of quantum mechanical calculations, several materials where a metal or heavy element substitutes an atom in a known semiconductor with appropriate band gap, creating inside the band gap a partially filled band2. This new intermediate band, allows the absorption of low energy photons inside the gap increasing the photo-current and also maintaining the photo-voltage. We present here compounds derived from different families of chalcogenides semiconductors, mainly chalcopyrites and spinels thin film and layered compounds: - Transition metal substituted CuGaS2 or similar chalcopyrite, where the thermodynamics of formation is seen to be less favourable than e.g. insertion of Mn in GaAs3. - In2S3 and other sulphides containing octahedral In. The V-doped In2S3 material is particularly promising. We have synthesized it in nanocrystalline form and shown that its optical absorption spectrum has the features predicted by quantum calculations4. Recent photocatalytic tests made with it show that the V dopant extends its spectral response down to the IR range without increasing recombination. - Octahedral SnIV sulphide and other similar compounds show also, according to theoretical modeling the formation of an IB with the desired characteristics when transition metals are introduced at Sn sites. The experimental synthesis of such sulphide show optical absorption spectra matching again the expectations for an IB material5. - In Si heavily doped with Ti, the desired IB electronic structure appears if Ti lies at interstitial sites. Such material has been prepared by ion implantation methods and its electrical properties show uncommon features explained by the formation of an IB as predicted by the DFT calculations. We also show that substitution of Si by S or Se, accompanied by hole doping, provides an IB material as well6. An overview of these systems, including results obtained on them using high level, state-of-the-art quantum calculation methods will be presented. Experimental results obtained for such novel IB materials matching in all cases the theoretical predictions7. *Presenter/corresponding author: perla@etsit.upm.es References 1. A. Luque and A. Martí, Phys. Rev. Lett. 78 (1997) 5014 2. P. Palacios et al. Phys. Rev. B 73 (2006) 085206; ibid. J. Chem. Phys. 124 (2006) 014711 3. P. Palacios et al. Thin Solid Films 515 (2007) 6280; ibid. J. Phys. Chem. C 112 (2008) 9525 4. P. Palacios et al. Phys. Rev. Lett. 101 (2008) 046403 ; R. Lucena et al. Chem. Maters. 20 (2008).

Auditorio-IFUAP
Lunes 25 de Agosto de 2014
12:00 Hrs.