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

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The intermediate band (IB) solar cell has been proposed as a novel device structure which could enhance photovoltaic efficiency, thanks to the cooperation of two sub-bandgap energy photons which allows the full excitation of an electron across the whole bandgap of a semiconductor[1]. 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 band[2]. 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 sulphides semiconductors, mainly spinels thin film and layered compounds:

- In_2S_3 and other sulphides containing octahedral In. The V-doped In_2S_3 material is particularly promising. We have synthesized it in nanocrystalline form and shown that its optical absorption spectrum has the features predicted by quantum calculations[3]. Recent photocatalytic tests made with it show that the V dopant extends its spectral response down to the IR range without increasing recombination.

- Octahedral Sn^{IV} layered 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 Van der Waals cleavage plane (0001) of these layered semiconductors is characterized by hexagonal arrays of close packed chalcogenide ions which are covalently bound within X-M-X sandwiches. This is an ideal substrate to study fundamental aspects of the metal/semiconductor interaction. The experimental synthesis of such sulphide show optical absorption spectra matching again the expectations for an IB material[4].

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 predictions.

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