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The double life of kesterite nanoparticles: photovoltaics and photocatalysis

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In the last decade, kesterite (Cu_2ZnSnS_4 – CZTS) thin films have been widely studied for photovoltaics (PV), due to their similarity to the well-known and well-performing $Cu(In,Ga)Se_2$ (CIGS). Its high absorption coefficient (> 10^4 cm^{-1}), its high stability and a tuneable direct band gap of 1.45 - 1.50 eV, promote kesterite as an ideal candidate for non-toxic, cheap, earth-abundant photovoltaic thin-film absorber.

Here we present our study on the properties and the possible use of CZTS in the form of nanoparticles (NPs) based on a straightforward hot-injection synthesis in an oxygen-free environment, starting from metal acetates and elemental sulphur in oleylamine. The impact of different injection temperatures on the crystalline size, crystal structure and formation of undesired secondary phases was investigated, along with a procedure to get rid of them. The resulting NPs were fully characterised by Raman spectroscopy, X-ray diffraction, energy-dispersive X-ray spectroscopy, transmission electron microscopy, and scanning electron microscopy. Additionally, the presence and removal of both organic traces and detrimental phases were confirmed by thermogravimetric analysis and FTIR-ATR analysis.

Our CZTS NPs were tested as potential inorganic hole transport material (HTM) to achieve cost-effectiveness, long-term operational stability and sustainability goals in perovskite solar cells (PSCs), especially if compared to the organic, expensive, not-sustainable but conventionally-used HTMs in PSCs (i.e. PTAA, 2PACz, PEDOT:PSS). The hole mobility and charge transport properties were investigated in plane and out of plane, to ensure the feasibility of the material to act as HTM. The resulting HTM film was used in p-i-n architecture with $[CH_3NH_3]PbI_3$ and compared to an organic-HTM-containing reference device. Under optimised conditions, the PSCs with CZTS NPs HTM remained stable, with PV performance improving by up to 80% of the initial value over time.

Parallelly, the photocatalytic activity of our CZTS NPs was tested, to address the environmental impact of industrial wastewater. To this purpose, the CZTS NPs were employed to degrade diclofenac (DCF) in water, being one of the most persistent and hazardous emerging micropollutants. Notably, the CZTS NPs show promising efficiency of 80-90% DCF degradation over 120 minutes in both UV-vis and Visible-light-only conditions, demonstrating its potential employment also in this field of application.