Exfoliated MoS₂ flakes as hole transport layer in perovskite-based photovoltaics

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Perovskite solar cells (PSCs) are emerging as the most promising next-generation photovoltaic technology because of their high power conversion efficiency (PCE) and low-cost. PSCs can be fabricated with simple procedures[1-3] and their maximum PCE has already exceeded 20%[4]. A planar PSC is usually composed of a glass substrate covered by a transparent conductive oxide (TCO), e.g., indium tin oxide (ITO), or fluorine-doped tin oxide (FTO), an electron conductive layer (e.g., TiO₂), a metal-organic perovskite photoactive layer (i.e., CH₃NH₃PbI₃), a hole transport layer (HTL) and a metal electrode, such as Ag or Au. The HTL is a crucial component that strongly affects the cell performance. Several materials have been proposed to work as HTL in PSCs, such as Spiro-OMeTAD, PEDOT:PSS, etc.[5] However, most of them have several issues such as stability, high production cost and low conductivity. For example, Spiro-OMeTAD needs a doping treatment to increase its hole conductivity. However, the dopants tend to desorb gradually from the Spiro-OMeTAD, strongly reducing the η of PSCs[1,6].

Here, we present a new HTL based on molybdenum disulfide (MoS₂) flakes. MoS₂ was chosen because of its chemically inertness, good electron mobility (~200cm² V⁻¹ s⁻¹), and an appropriate energy level (5.2eV, close to the perovskite's valence band of 5.0eV)[1]. MoS₂ bulk crystals are exfoliated in 2-propanol and deposited on perovskite layers by spray coating[7,8]. The characterization of the liquid dispersion indicates that the MoS₂ flakes are composed of few layers. The TEM analysis in Fig.a shows the presence of exfoliated flakes with a lateral size in the order of 100-200nm. The electron diffraction pattern (Fig.a, inset) shows the hexagonal crystalline structure characteristic of MoS₂ flakes. A comparative study between PSCs made with MoS₂ and un-doped Spiro-OMeTAD shows that the cell with MoS₂ has higher open-circuit voltage (0.74V vs 0.56V) and fill factor (72% vs 51%). The MoS₂-based PSCs (see Fig. b) show an increase in the PCE values with respect to the PSCs based on the un-doped Spiro-OMeTAD cell (3.9% vs 3.1%). Shelf-life test shows no PCE degradation in the first 800 hours. These results represent a step forward towards the fabrication of PSCs with a simple and economic approach for the industrial production of stable and efficient photovoltaic devices.

References

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Figures



Fig. a) TEM image of exfoliated MoS₂ flakes. Inset: electron diffraction pattern. **b)** I/V characteristics of perovskite-based cells with MoS₂ flakes as HTL and with pristine Spiro-OMeTAD.