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Bismuth iron tungstate pyrochlore thin films for photovoltaic applications

Sergey S. Kozlov, Anna B. Nikolskaia, Olga V. Alexeeva, Ekaterina K. Kosareva, Oksana V. Almjasheva, Viktor V. Gusarov, Oleg I. Shevaleevskiy and Liudmila L. Larina

S1. Experimental

1.1. Fabrication of BFWO nanopowders

The BFWO nanopowders were obtained by hydrothermal synthesis according to procedure described in [1]. $Bi(NO_3)_3 \cdot 5H_2O$ (2 mmol) and $Fe(NO_3)_3 \cdot 9H_2O$ (1.44 mmol) were dissolved in 30 ml of 1M HNO_3. $Na_2WO_4 \cdot 2H_2O$ (4 mmol) was dissolved in 30 ml of distilled water and then added dropwise to the stirred acidic solution of bismuth and iron nitrates. After 1 hr of continuous stirring of the resulting suspension, a solution of NaOH 4M was added dropwise to obtain pH value of 2. After additional stirring for ~1 hr, precursor was relocated to a steel autoclave and placed in an oven heated up to 200 °C. After 24 h, the autoclave was removed from the oven and cooled in air at room temperature. The resulting precipitate was separated from the mother liquor by centrifugation, rinsed with distilled water, and dried in air at 80 °C for 20 h.

1.2. Fabrication of PSCs

The BFWO nanopowder was mixed with acetic acid, terpineol, ethyl cellulose and ethanol to obtain thick paste as specified in [2]. This paste was diluted in ethanol (1:5), sonicated in ultrasonic bath several times and was deposited by spin coating (3000 rpm, 30 s) onto FTO (fluorine doped SnO_2) conductive glass substrates (Solaronix, 2×2 cm) with subsequent annealing at 500ºC in air for 1 hr. Thus, the mesoporous ETL thin films based on BFWO was obtained. State-of-the-art TiO_2-based ETL thin film was fabricated using the same technique for comparative analysis [2].

PSCs were fabricated under ambient conditions at relatively high humidity (~50-60%) according to the procedure described in [2]. The solution of perovskite $CH_3NH_3PbI_3$ was prepared by mixing 461 mg PbI_2, 159 mg CH_3NH_3I and 71 μl DMSO in 635 μl of DMF (a molar ratio of 1:1:1). This solution was spin-coated on the ETL surface at 4000 rpm for 25 s by a one-step deposition method using diethyl ether as antisolvent. Obtained perovskite layers were dried at 100ºC for 10 min. At the next step, the hole-transporting material Spiro-MeOTAD was deposited by spin-coating at 2000 rpm for 30 s. The following solution was used: 72.3 mg Spiro-MeOTAD,

28.8 µl 4-tert-butylpiridine and 17.5 µl Li-TFSI solution (520 mg Li-TSFI in 1 ml of acetonitrile) in 1 ml of chlorobenzene. The process of PSC fabrication was completed by the deposition of the Au electrodes with a thickness of 50 nm using vacuum thermal evaporation with the VUP-4 vacuum post. The structure of the PSC with BFWO-based ETL is shown on Figure S1.

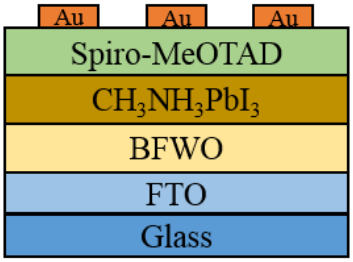

Figure S1 The structure of BFWO-based PSC.

1.3. Characterization studies

The optoelectronic properties of BFWO powders were characterized using UV-vis spectroscopy (Shimadzu UV-3600 spectrophotometer with an ISR-3100 integrating sphere in the wavelength range of 300-1200 nm). AFM data were obtained using atomic-force microscope NTEGRA Prima (NT-MDT, Zelenograd, Russia). The PV measurements for PSCs fabricated were provided under standard illumination conditions of 1000 W/m^2 (AM1.5G) using Abet 10500 solar simulator (Abet Technologies, USA). The current density–voltage (J–V) characteristics were measured by Semiconductor Characterization System 4200-SCS (Keithley, USA). PSCs were masked to obtain working area of 0.08 cm^2.

References

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S2. Supplementary data

Table S1 PV characteristics of the PSCs with different ETLs.

Type of ETL	J_{SC}, mA/cm^2	V_{OC}, V	*FF*, a.u.	PCE, %
TiO_2	18.8 ± 0.18	1.00± 0.02	0.69 ± 0.02	12.8 ± 0.17
BFWO	20.5 ± 0.17	0.89 ± 0.01	0.73 ± 0.01	13.3 ± 0.15