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Understanding the Impact of Li- bis(trifluoromethanesulfonyl)imide Doping on Spiro-OMeTAD Properties and Perovskite Solar Cell Performance

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Abstract : Lithium bis(trifluoromethanesulfonyl)imide (Li-TFSI) dopant is beneficial in improving the properties of 2,2′,7,7′-Tetrakis (N, N-di-p-methoxyphenylamino)-9,9′-spiro-bifluorene (Spiro-OMETAD) transport layer used in perovskite solar cells (PSCs). Properties such as electrical conductivity, band energy mismatch, and refractive index of Spiro-OMETAD layers are believed to play key roles in PSCs performance but only the dependence of electrical conductivity on Li-TFSI doping has been extensively studied. In this work, the effect of Li-TFSI doping level on highest occupied molecular orbital (HOMO) energy, electrical conductivity, and refractive index of Spiro-OMETAD film and PSC performance was demonstrated. The Spiro-OMETAD films were spin-coated at 4000 rpm for 30 seconds from solutions containing 73.4 mM of Spiro-OMeTAD, 23.6 mM of 4-tert-butylpyridine, 7.6 mM of tris(2-(1H-pyrazol-1-yl)-4-tert-butylpyridine) cobalt(III) tri[bis(trifluoromethane) sulfonimide] (FK209) dopant and Li-TFSI dopant varying from 37 to 62 mM in 1 ml of chlorobenzene. From ultraviolet photoelectron spectroscopy (UPS), ellipsometry, and 4-probe studies, the results show that films deposition from Spiro-OMETAD solution doped with 40 mM of Li-TFSI shows the highest electrical conductivity of 6.35×10-6 S/cm, the refractive index of 1.87 at 632.32 nm, HOMO energy of -5.22 eV and the lowest HOMO energy mismatch of 0.21 eV compared to HOMO energy of perovskite layer. The PSCs fabricated show the best power conversion efficiency, open-circuit voltage, and fill factor of 17.10 %, 1.1 V, and 70.12%, respectively, for devices based on Spiro-OMETAD solution doped with 40 mM of Li-TFSI. This study demonstrates that the optimum Spiro-OMETAD/ Li-TFSI doping ratio of 1.84 is the optimum doping level for Spiro-OMETAD layer preparation.

Keywords : electrical conductivity, homo energy mismatch, lithium bis(trifluoromethanesulfonyl)imide, power conversion efficiency, refractive index
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