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Original Paper

Self-passivation of molecular n-type doping during air exposure using a highly efficient air-instable dopant

Max L. Tietze , Florian Wölzl, Torben Menke, Axel Fischer, Moritz Riede, Karl Leo , Björn Lüssem

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Abstract

In contrast to p-dopants, highly efficient molecular n-dopants are prone to degradation in air due to their low ionization potentials, limiting the processing conditions of doped functional organic devices. In this contribution, we investigate the air-stability of pure films of the n-dopant tetrakis(1,3,4,6,7,8-hexahydro-2H-pyrimido[1,2-a]pyrimidinato)ditungsten(II) ($W_2(hpp)_4$) and of C_{60} layers doped by $W_2(hpp)_4$. We find that 1/3 of the initial conductivity of the doped C_{60} thin films can be restored by thermal annealing in vacuum after a drop by 5 orders of magnitude upon air exposure. Furthermore, we show by ultraviolet photoelectron spectroscopy (UPS) and Seebeck measurements that the Fermi level shift toward the lowest unoccupied molecular orbital (LUMO) of C_{60} remains after air exposure, clearly indicating a conservation of n-doping. We explain these findings by a down-shift of the $W_2(hpp)_4$ energy levels upon charge-transfer to a host material with deeper lying energy-levels, facilitating a protection against oxidation in air. Consequently, the observed recovery of the conductivity can be understood in terms of a self-passivation of the molecular n-doping. Hence, an application of highly efficient n-doped thin films in functional organic devices handled even under ambient conditions during fabrication is feasible.

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