NOVEL CARBORANE-BASED ELECTRON-TRANSPORTING MATERIALS FOR PEROVSKITE SOLAR CELLS

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Lead-based halide perovskite solar cells (PSCs) have gained significant attention due to their rapid performance advancements, with certified power conversion efficiencies (PCE) now reaching up to 27.3%, making them comparable to silicon solar cells. Recently, a perovskite/silicon tandem solar cell efficiency of 35.0% was reported, which exceeds the theoretical efficiency limit of 29.5% for a silicon single-junction cell [1]. Buckminsterfullerene (C_{60}) is the standard electron-transporting layer (ETL) used in high-efficiency p-i-n perovskite single-junction and perovskite/silicon tandem solar cells, owing to its ability to rapidly extract electrons from the perovskite absorber [2, 3], its relatively high electron mobility, and compatibility with thermal evaporation allowing for the deposition of thin, conformal layers over large substrate areas. However, C_{60} has several disadvantages such as high cost, interfacial non-radiative recombination, high parasitic absorption, and poor mechanical stability at the interface with the perovskite absorber as well as the SnO_x layer on top leading to interfacial delamination. Organic electron-transporting materials (ETMs) have recently attracted much attention as an alternative to fullerene C_{60} due to their low cost, straightforward synthesis as well as better adhesion with perovskite.

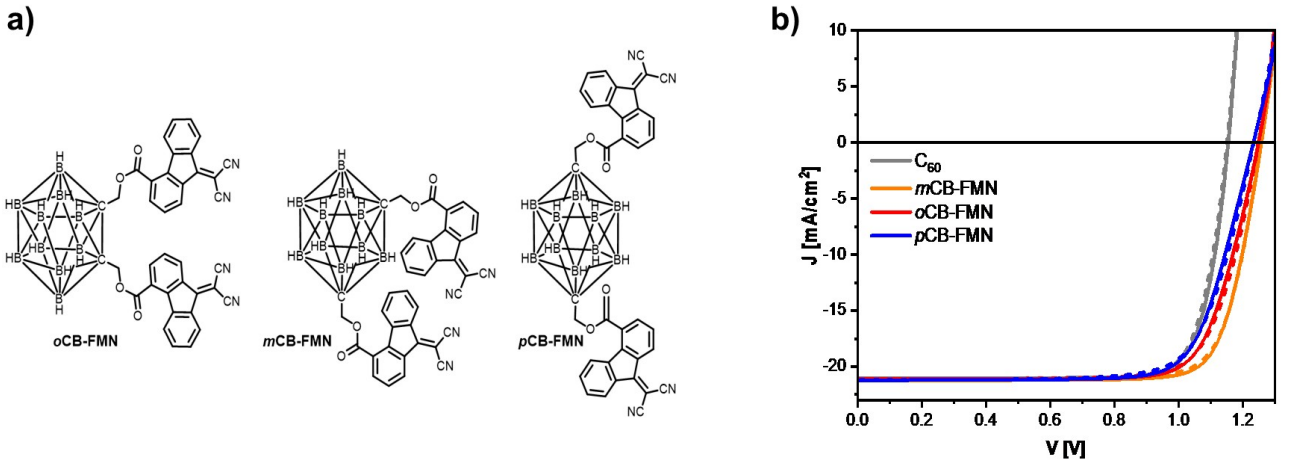

Fig. 1. a) The structures of carborane-based ETMs; **b)** *J-V* characteristics.

In this work, fluorenylidene malononitrilesubstituted carborane derivatives were synthesized and investigated as non-fullerene ETM for perovskite-based solar cells. Charge mobility of the layers based on o,m,p-series carborane derivatives was determined by xerographic time-of-flight (XTOF) measurements. The samples for the measurements were prepared by evaporating carborane compounds on polyester films with conductive Al layer. As a result, the electron mobility of **oCB-FMN**, **mCB-FMN** and **pCB-FMN** was found to be 1×10^{-5}, 5×10^{-5}, and 5×10^{-6} cm^2/Vs at zero-electric field. The new materials were tested as ETMs and successfully applied in single-junction PSCs. During device fabrication all ETMs were deposited by thermal evaporation. Furthermore, *m*-carborane derivative demonstrated best performance exhibiting a PCE 21.4% and revealing an efficiency potential that surpasses control devices with C_{60}. The new carborane derivatives demonstrate lower interfacial non-radiative recombination losses and reduced parasitic absorption in tandem devices for wavelength shorter than 650 nm, which highlights their potential as alternatives to C_{60}.

[1] "Best Research-Cell Efficiency Chart | Photovoltaic Research | NLR." https://www.nrel.gov/pv/cell-efficiency.html
[2] J. Siekmann et al., "Characterizing the influence of charge extraction layers on the performance of Triple-Cation perovskite solar cells," Advanced Energy Materials, vol. 13, no. 32, Jul. 2023, doi: 10.1002/aenm.202300448.
[3] Z. Guan et al., "Ultrafast Electron-Transfer via hybrid states at Perovskite/Fullerene Interface," Advanced Materials, vol. 36, no. 38, p. e2407406, Jul. 2024, doi: 10.1002/adma.202407406.