

Supplementary Information

Novel Carbazole-Acridine-Based Hole Transport Polymer for Low Turn-on Voltage of Green Quantum Dot Light-Emitting Diodes

Chai Won Kim,^a Ji Hye Lee,^a Seunguk Cho,^a Hyung Jong Kim,^a Jinhyo Hwang,^a Yong Woo Kim,^b Dae Hyuk Choi,^b Min Ju Cho,^{a*} Kwangyeol Lee,^{a*} and Dong Hoon Choi^{a*}

^a Department of Chemistry, Research Institute for Natural Sciences, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul, 02841, Republic of Korea.

^b LT Materials, 113-19, Dangha-Ro, Namsa-Myeon, Cheoin-Gu, Yongin-Si, Gyeonggi-Do 17118, Republic of Korea

* Corresponding authors: M. J. Cho (chominju@korea.ac.kr); K. Lee (kylee1@korea.ac.kr); D. H. Choi (dhchoi8803@korea.ac.kr)

Experimental

Instrumentation

¹H nuclear magnetic resonance (NMR) spectra were recorded using Varian Mercury 500-MHz spectrometers in CDCl₃ solvent. Mass spectrometry was performed using a MALDI-TOF MS instrument (Bruker Daltonics). Differential scanning calorimetry (DSC, Mettler 821 Instrument) was performed to observe the thermal properties of the hole transport materials (HTMs). Elemental analysis was conducted using a FlashSmartTM elemental analyzer.

The absorption spectra of the HTMs were obtained using a UV-vis spectrophotometer (HP 8453, $\lambda = 190\text{--}1100$ nm), and Photoluminescence (PL, Hitachi F-7000 and Thermo FA-357 fluorescence spectrophotometer) spectra were recorded at room temperature (298 K). To measure the oxidation potential of the HTMs in the film state, cyclic voltammetry (CV) analysis was performed at a scan rate of 50 mV s⁻¹ using a potentiostat (EA161, eDAQ). UV photoemission spectroscopy (UPS, Nexsa XPS system) was performed to find the energy

levels of the HTMs with He I as the UV source (21.2 eV). The samples were prepared in the film state, and the base pressure for the instrument was 2.0×10^{-7} Torr.

Space-charge-limited current (SCLC) method for measuring hole mobility

The hole mobilities of the HTMs were measured using the SCLC method after the fabrication with a typical device structure comprising of ITO/PEDOT:PSS (20 nm)/PVK or **P-CzAc** film (100 nm)/MoO₃ (10 nm)/Ag (100 nm). The mobility was calculated according to $J = 9\epsilon_0\epsilon_r\mu V^2/8L^3$, where J is the current density, ϵ_0 is the permittivity of the HTL, ϵ_r is the relative dielectric constant, μ is the hole mobility, and L is the thickness of the HTL. The internal voltage is $V = V_{\text{appl}} - V_{\text{bi}} - V_{\text{a}}$, where V_{appl} is the voltage applied to the device, V_{bi} is the work function difference between two electrodes, and V_{a} is the voltage drop.

Green QD-LED Fabrication and Measurements

The green QD-LED device structure comprised ITO/PEDOT: PSS (20 nm)/HTL (PVK (20 nm) or **P-CzAc** (20 nm))/EML (QD: CdSe@ZnS core-shell structure, 10 mg/mL in octane)/Zn_{0.85}Mg_{0.15}O (30 nm)/Al (100 nm). Prior to device fabrication, the ITO-coated substrates were washed with deionized water and isopropanol under ultrasonication for 10 min. Initially, UV-ozone treatment was performed for 20 min and PEDOT: PSS (20 nm) was deposited on the ITO-coated substrates at a spin rate of 4000 rpm for 40 s, followed by annealing at 155 °C for 15 min. Subsequently, the substrate was placed in a nitrogen-filled glove box. Then, 1.0 wt.% PVK [Tokyo Chemical Industry, $M_n = 60.0$ kDa] solution was prepared from a chlorobenzene solvent, spin-coated on top of the ITO/PEDOT: PSS, and subsequently annealed at 130 °C for 20 min. The emitting layer was prepared from an octane solution of

CdSe@ZnS QDs and spin-coated at 3000 rpm for 30 s. Zn_{0.85}Mg_{0.15}O with a thickness of 30 nm was deposited at 3000 rpm for 30 s and annealed for 15 min at 120 °C. Finally, Al electrodes were fabricated by vacuum deposition. The QD-LED device characteristics were measured using a Keithley SMU 236 instrument and a SpectraScan PR-655 colorimeter.

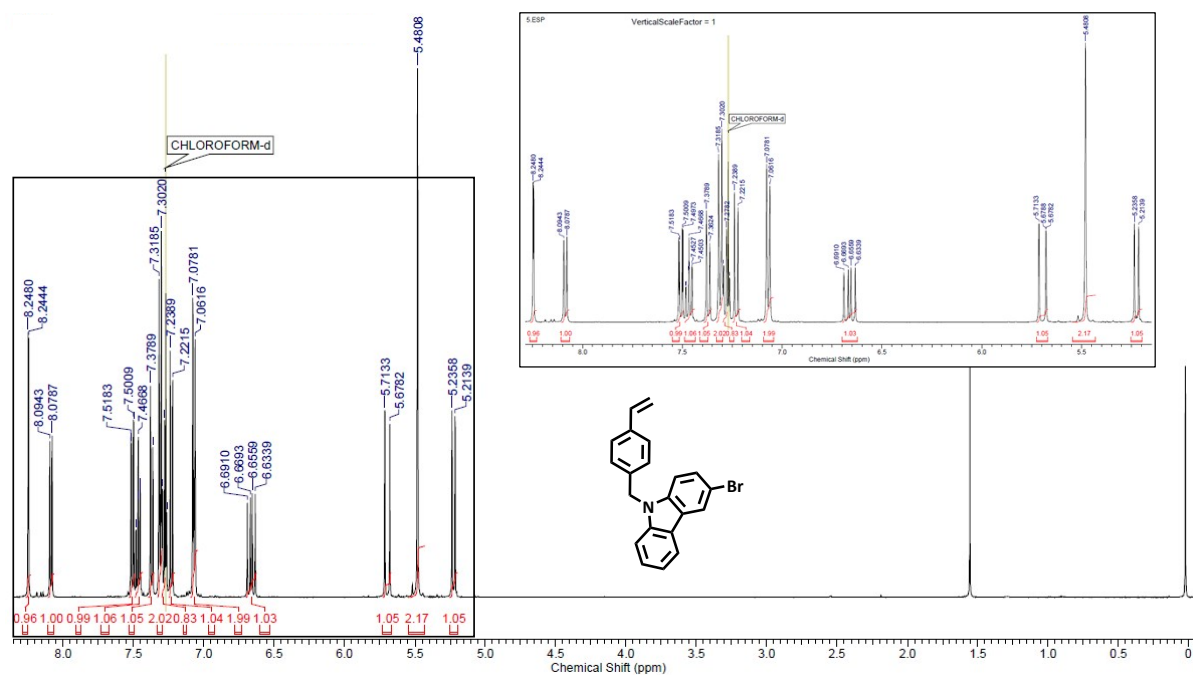


Fig S1. ¹H NMR spectrum of 3-bromo-9-(4-vinylbenzyl)-9H-carbazole.

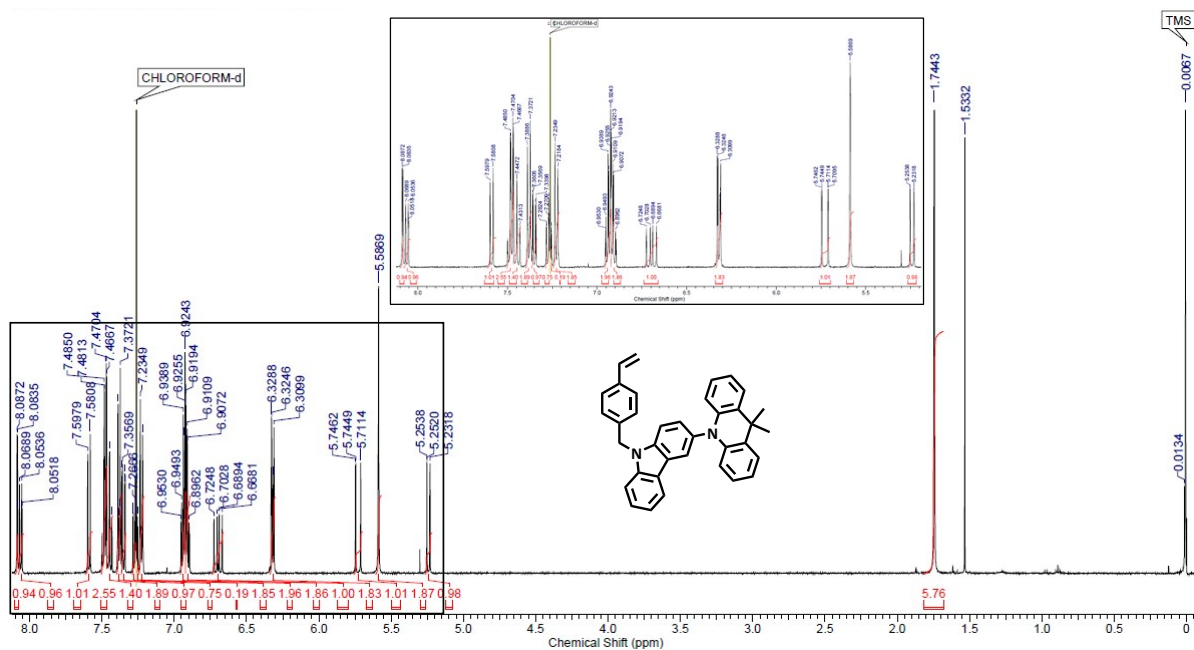


Fig S2. ^1H NMR spectrum of 9,9-dimethyl-10-(9-(4-vinylbenzyl)-9H-carbazol-3-yl)-9,10-dihydroacridine.

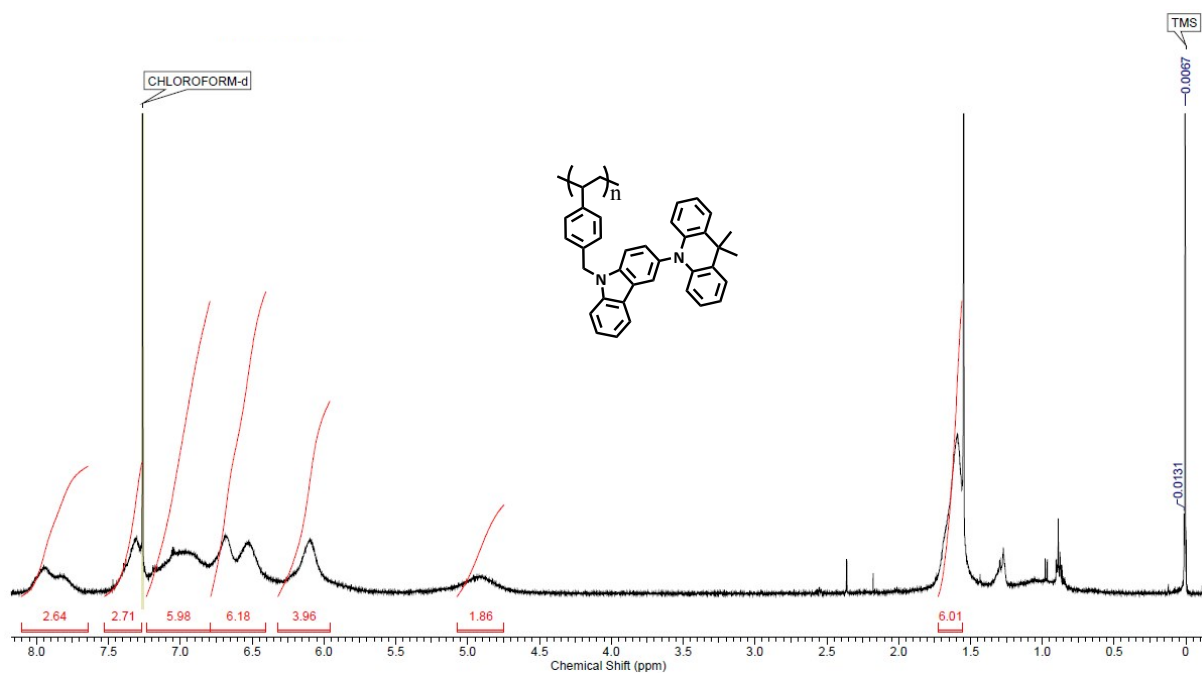


Fig S3. ^1H NMR spectrum of P-CzAc.

S

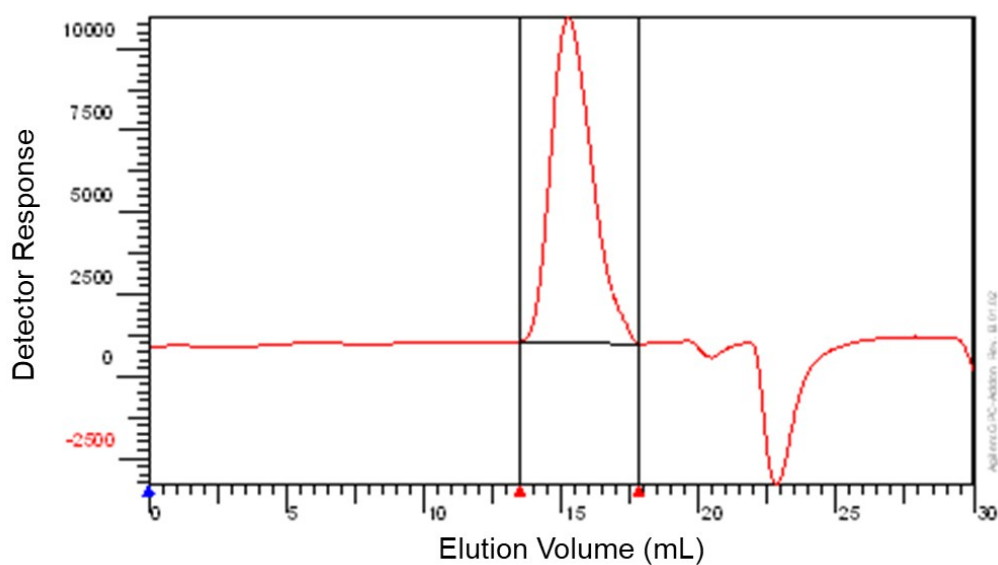


Fig. S4. GPC analysis of **P-CzAc**.

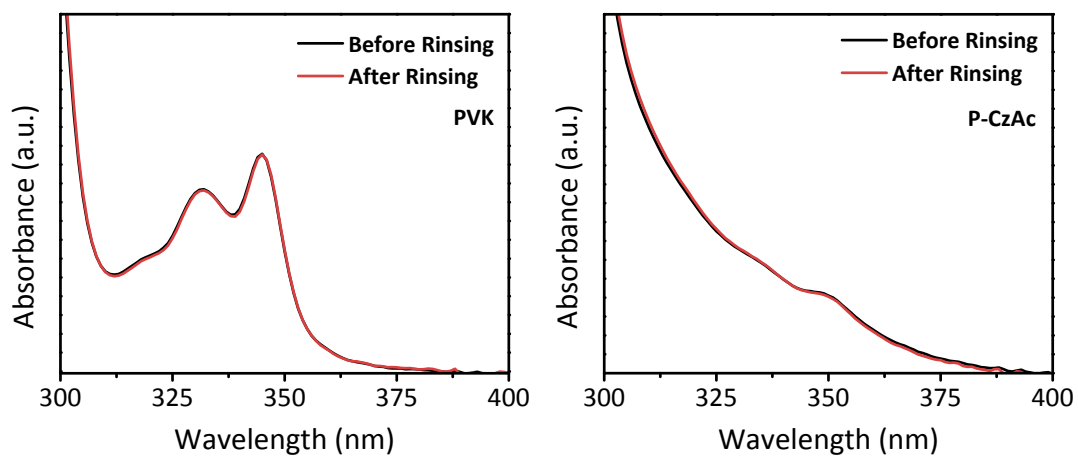


Fig. S5. Absorption spectra of PVK and **P-CzAc** in thin film states prior to and following solvent rinsing.

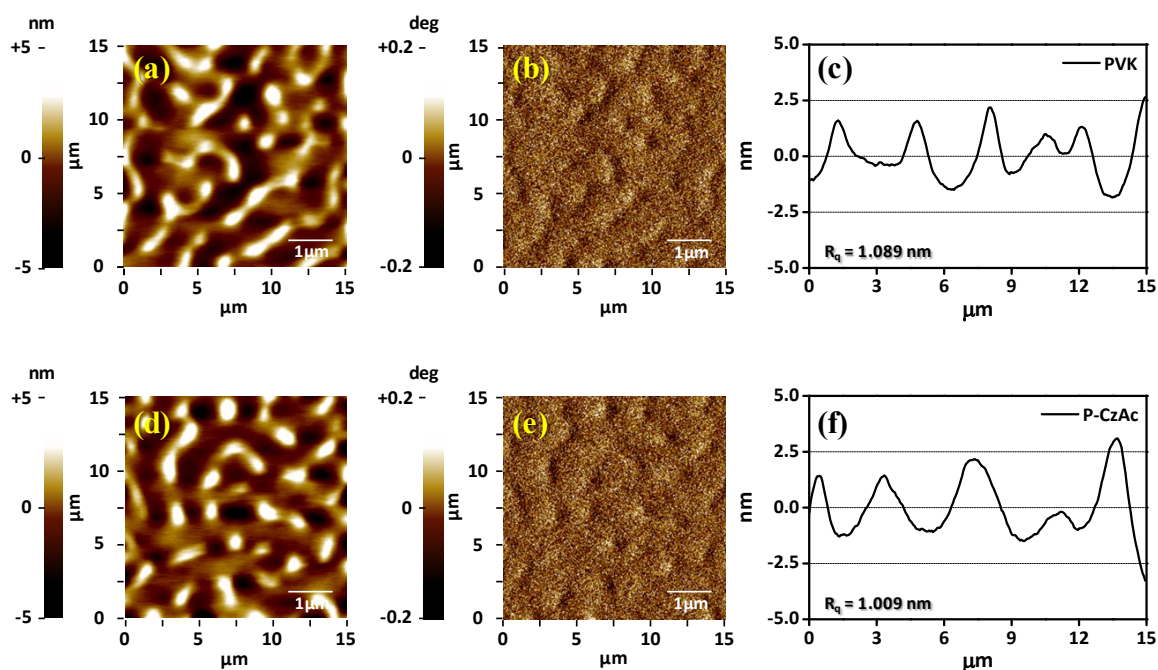


Fig. S6. AFM topography (a, d), phase (b, e) images (15 μm × 15 μm), and line profile (c, f) of QD layer on PVK (a, b, c) and P-CzAc (d, e, f) HTL.

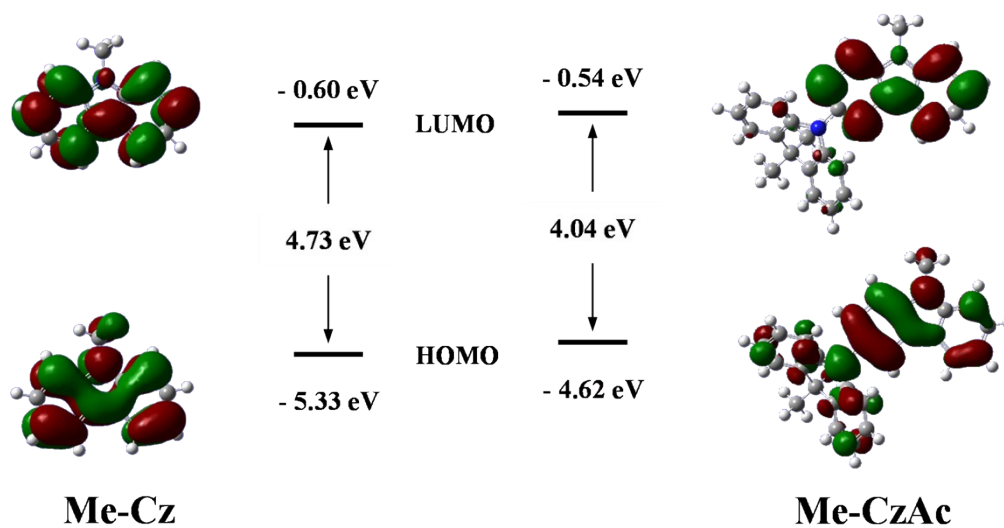


Fig. S7. Optimized structures and HOMO and LUMO distributions of simplified PVK and P-CzAc by B3LYP in DFT calculations.