

Defect chemistry of polyfluorenes: Identification of the origin of “interface defects” in polyfluorene based light-emitting devices

Stefan Kappaun,^{*a,×} Horst Scheiber,^{b,c,×} Roman Trattnig,^{b,c} Egbert Zojer,^b Emil J. W. List^{a,b,c} and Christian Slugovc^d

^a NanoTecCenter Weiz Forschungsgesellschaft mbH, Franz-Pichler-Straße 32, A-8160 Weiz

^b Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz

^c CD-Labor Advanced Functional Materials, Graz University of Technology, Petersgasse 16, A-8010 Graz

^d Institute for Chemistry and Technology of Materials (ICTM), Graz University of Technology, Stremayrgasse 16, A-8010 Graz

[×] These authors contributed equally to the work.

*email: stefan.kappaun@ntc-weiz.at, phone: ++43 (0)316 876 8015, fax: ++43 (0)316 876 8040

Electronic Supplementary Information

Experimental section

Titration experiments in solution. UV-Visible absorption spectra were recorded on a Cary 50 Bio UV-Visible Spectrophotometer, fluorescence spectra on a Perkin Elmer Luminescence Spectrometer LS50B. All measurements were conducted under ambient conditions.

Thin film spectra. Thin film photoluminescence spectra of **1** were recorded using an ORIEL spectrometer with an attached ANDOR DB401-UV CCD camera corrected with the corresponding response curve of the detector. The 364 nm line of a COHERENT INNOVA 300 argon ion laser was used as excitation source for photoluminescence measurements. All measurements were conducted under inert atmosphere of argon.

Titration experiments of **1**, **2** and **3** in solution

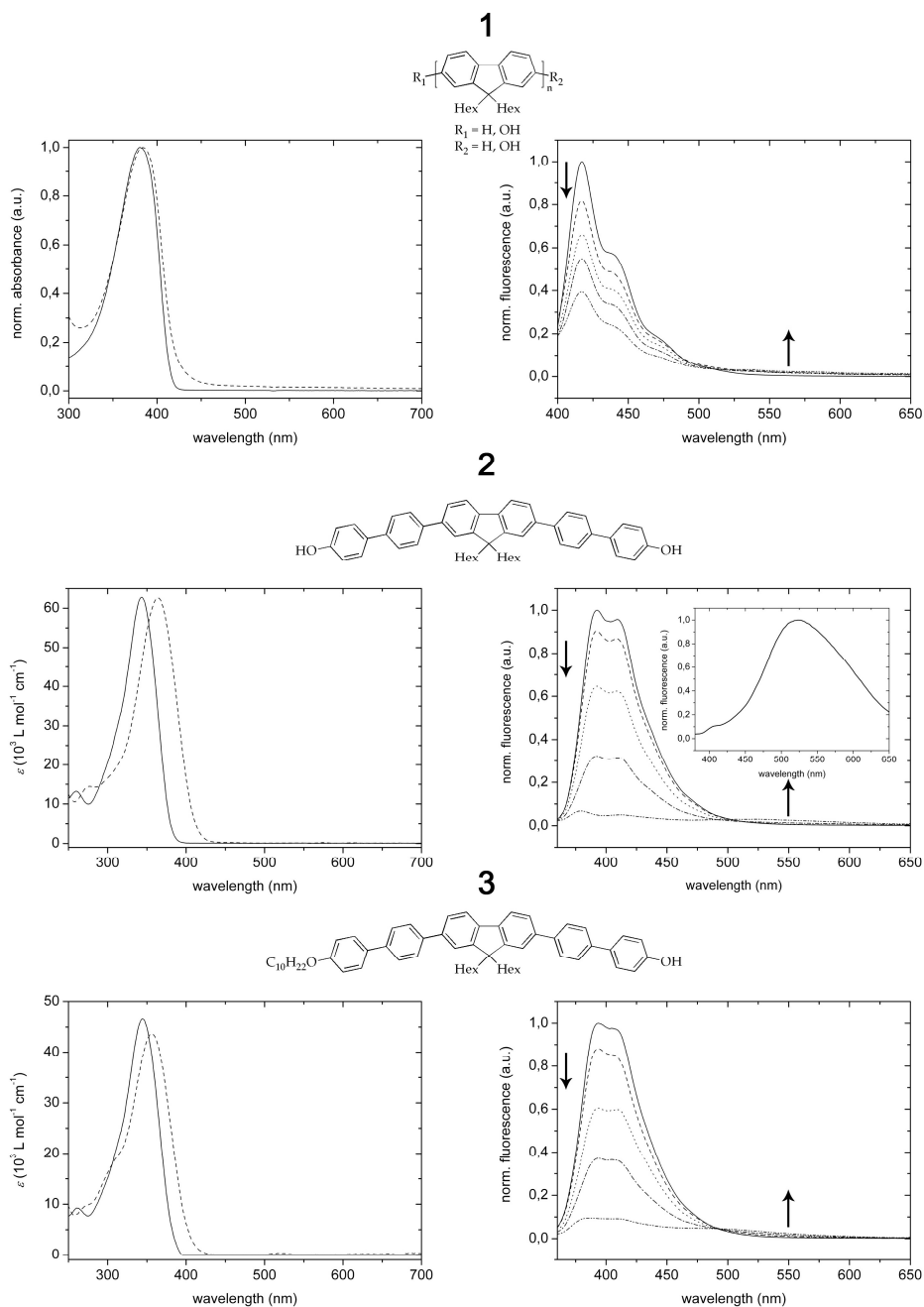
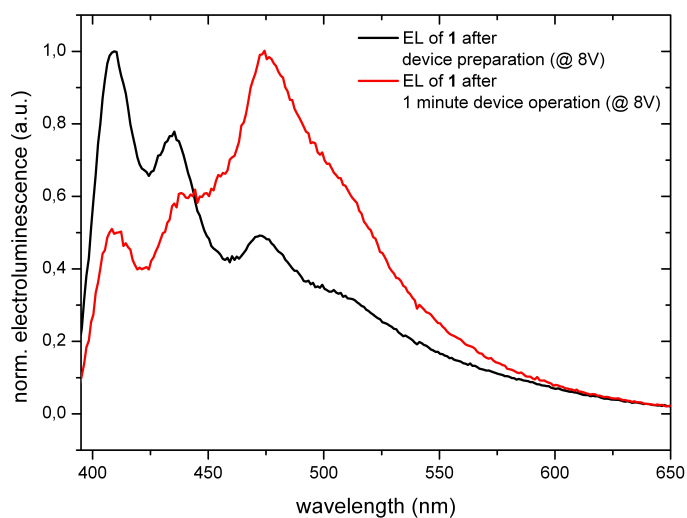


Figure ESI1. Titration experiments of **1**, **2** and **3** show a drastic decrease of the blue emission peak upon addition of a strong base with simultaneous increase of a new, red-shifted emission band (very weak emission intensity in solution). While also the corresponding absorption maxima are red-shifted in case of **2** and **3**, the absorption spectrum of **1** remains virtually unchanged upon addition of a strong base.

a)



b)

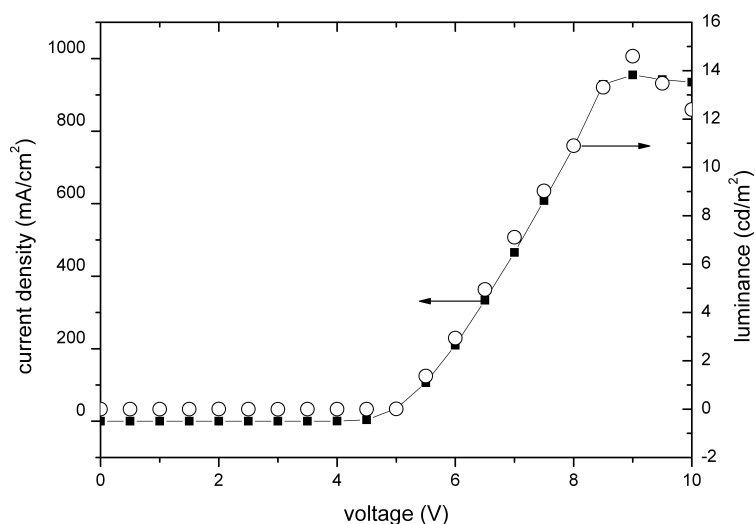


Figure ESI2. a) Electroluminescence spectra of a PLED prepared with the hydroxy terminated polyfluorene **1** (ITO/PEDOT:PSS/1/Ca/Al). While the blue electroluminescence is just observed for a few seconds after device turn-on, interface defects dominate the electroluminescence spectrum after (in maximum) 1 minute. Devices with hydrogen terminated polyfluorenes show increased device stabilities (green emission from keto defect sites after some minutes). b) Device characteristics of a PLED prepared with the hydroxy terminated polyfluorene **1** (ITO/PEDOT:PSS/1/Ca/Al).

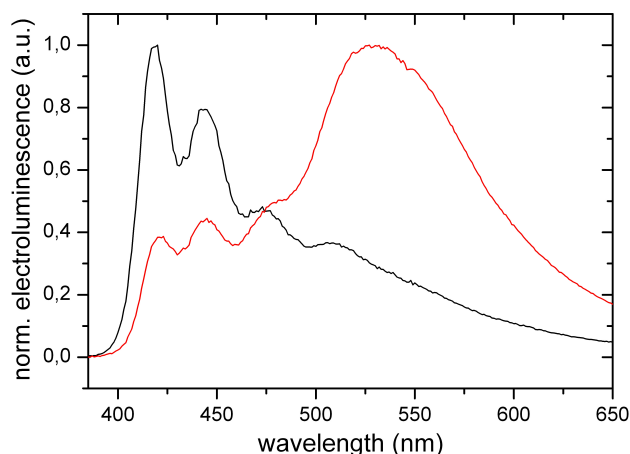


Figure ESI3. Electroluminescence spectra of hydrogen terminated polyfluorenes before (black line) and after degradation (red line). Here, the greenish emission colour (emission maximum around 550 nm) stems from ketonic defect sites.

Comparing Figure ESI2 and ESI3 significant differences concerning the emission maxima become evident. While in case of hydroxy terminated polyfluorenes (cf. Figure ESI2) the green emission band peaking around 500 nm can be explained with deprotonation effects, the green electroluminescence of hydrogen terminated polyfluorenes (cf. Figure ESI3) is a result of ketonic defect sites generated during polymer synthesis and/or device degradation.

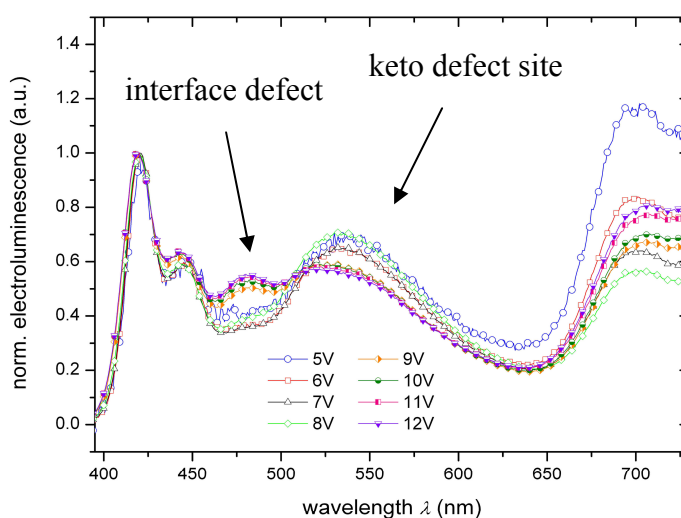


Figure ESI4. The green emission peak around 500 nm is frequently observed in polyfluorene based PLEDs. Here, the EL spectrum of a white polymeric light-emitting device (fluorene-iridium main chain polymer prepared *via* a Suzuki cross-coupling reaction) is shown also exhibiting this feature.^{ESI1}

^{ESI1} S. Kappaun, S. Eder, S. Sax, R. Saf, K. Mereiter, E. J. W. List and C. Slugovc, *J. Mater. Chem.*, 2006, **16**, 4389.