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In Silico Toxicity Screening as a Tool for the Development of Sustainable Electronics, Exemplified with Organic Light-Emitting Electrochemical Cells

Papri Sutar,[a] Thomas P. McGrath,[b] Kunal Lulla,[b] Christopher Somerton,[b] Mark D. Ashton,[a] Garry R. Harper,[a] Nathan R. Halcovitch,[a] Richard L. Mort,[c] Karen L. Wright,[c] Alison F. Stowell,[d, e] David Bird,[g] Robert J. Young,*[b] and John G. Hardy*[a, f]

Electrical and electronic equipment (EEE) have revolutionized our lives, however, their associated waste (WEEE) presents a global challenge because at this time EEE relies heavily on metals that are not commonly found in the living environment (Biosphere), which find their way into the environment during both production/disposal of EEE/WEEE. The use of organic components in EEE is increasingly common, particularly with the growing interest in flexible electronics. Here we describe an approach to device design employing *in silico* toxicity screening to assess the toxicity of the components chosen for use in EEE that is exemplified using inorganic and organic components known in the literature for the production of prototype organic light-emitting electrochemical cells. This approach could easily be employed to screen a variety of components for which datasets to produce safety data sheets (SDSs) don't yet exist because they have not been produced in large scale or in a regulatory environment which necessitates this. The approach has significant potential to improve high throughput screening of components for EEE that are "safe-by-design", potentially in combination with AI and ML approaches.

Introduction

EEE is ubiquitous in our lives, and is concomitantly manufactured at industrial scales to meet consumer demand (a multi-billion dollar industry worldwide).[1] Electronics manufacturers commonly require metals that are critical raw materials[1b] employ a variety of processes to produce complex devices from a host of materials (including conductors, semiconductors, resistors and non-conductors), in automated factories on rigid or flexible substrates, as necessitated by the application.[2] Current trends in the development and manufacture of electronics include miniaturization, use of new computational approaches (e.g., artificial intelligence (AI) and machine learning (ML)), use of new materials (e.g., organic electronics, 2D materials, flexible materials, etc.[3] and use of new manufacturing approaches (e.g., additive manufacturing, internet of things (IoT), mass customisation and personalisation).[4]

Electronics's pervasive roles in our lives leads to the generation of significant quantities of WEEE (also commonly known as e-waste) from the production and disposal of products (> 50 million tonnes of WEEE per year).[5] The quantity of WEEE increases annually in line with global efforts to reduce poverty, population growth, and the ever increasing use of electronic technologies in our lives.[6] WEEE is therefore an issue of global importance due to ecological concerns (e.g., air/soil/water pollution) from some of the components of WEEE and their impacts on veterinary/human health.[7]

The production of EEE happens worldwide in countries with significant differences in regulation. Indeed, in some countries safety data sheets (SDSs) listing information relating to the

[a] *P. Sutar, M. D. Ashton, G. R. Harper, N. R. Halcovitch, J. G. Hardy*
Department of Chemistry, Lancaster University, Faraday Building, John Creed Avenue, Lancaster, Lancashire LA1 4YB, UK
E-mail: j.g.hardy@lancaster.ac.uk
Homepage: https://www.lancaster.ac.uk/chemistry/about/people/john-george-hardy

[b] *T. P. McGrath, K. Lulla, C. Somerton, R. J. Young*
Department of Physics, Lancaster University, Faraday Building, Physics Avenue, Lancaster, Lancashire, LA1 4YW, UK
E-mail: r.j.young@lancaster.ac.uk
Homepage: https://www.lancaster.ac.uk/physics/about-us/people/robert-young

[c] *R. L. Mort, K. L. Wright*
Division of Biomedical and Life Sciences, Lancaster University, Tower Avenue, Lancaster, Lancashire LA1 4YG, UK

[d] *A. F. Stowell*
Department of Organisation, Work and Technology, Lancaster University, Lancaster University Management School, Lancaster, LA1 4YX, UK

[e] *A. F. Stowell*
Pentland Centre for Sustainability in Business, Lancaster University, Lancaster University Management School, Lancaster, LA1 4YX, UK

[f] *J. G. Hardy*
Materials Science Lancaster, Lancaster University, Lancaster, Lancashire, LA1 4YW, UK
E-mail: j.g.hardy@lancaster.ac.uk

[g] *D. Bird*
Centre for Process Innovation (CPI), Sedgefield, County Durham, TS21 3FG, UK

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hazards of working with a substance in an occupational setting, (particularly physico-chemical, health, or environmental risks) are mandatory. However, even though there is a Globally Harmonized System of Classification and Labelling of Chemicals which contains a standard specification for SDSs,[7f] the use of this system is not mandatory in every country meaning that it is possible for substances/products to enter global supply chains and/or the environment without a complete understanding of the risks associated with their production/disposal.

The development of EEE including new materials is popular because it offers opportunities to generate new intellectual property that can be harnessed in the production of new products. Early stage research happens on very small scales (relative to global production of EEE) including for new substances for which SDSs don't yet exist because they have not been produced in large scale or in a regulatory environment which necessitates this.

In silico toxicology is a type of toxicity assessment that employs computational methodologies to predict the toxicity of chemicals based on a combination of data analysis/simulation/visualization. It has been used to facilitate the development low molecular weight organic molecules for industrial applications including but not limited to agrochemicals and drugs. Consequently, the application of *in silico* toxicity prediction to the research and development of EEE offer an enriched understanding of the risks associated with the substances used, and has significant potential to improve high throughput screening of components for EEE that are "safe-by-design", potentially in combination with AI and ML approaches.

Light-emitting electrochemical cells (LECs) are a class of electroluminescent device that have a multitude of industrially relevant applications,[8] they are a potentially disruptive technology because they are recyclable, energy efficient and might overcome the problem of WEEE which is a major ecological threat and a risk to human health.[9]

Light-emitting materials can be used for a variety of technical and medical applications,[10] of which, light-emitting diodes (LEDs) are one example of devices composed of mixtures of inorganic and organic components, typically requiring controlled atmospheres and high energies when being manufactured,[11] however, low energy solution processing is an area of significant interest in academic and industry settings.[12] LECs are another example of light-emitting devices which are the subject of a number of excellent reviews,[13] including those exploring the variety of materials employed in their production.[14] and trends towards the development of flexible LECs,[15] that could be integrated in textiles,[16] and towards more environmentally friendly versions.[17]

The impact of artificial lighting is a major contributor to carbon emissions and the development of greener more efficient alternatives is an attractive means to address issues related to greenhouse gases and climate change. In the UK the National Health Service (NHS) has recognized that medical devices are a significant contributor to carbon emissions and as part of delivering a net zero NHS future procurement decisions will be based on the sustainability and the carbon footprint of medical devices.[18] In essence, this means that devices that contain sustainable technologies, will have significant competitive advantage over those that don't. Therefore, at least in the health sector, there are real commercial procurement drivers that should drive adoption of devices that contain OLEC based technology.

Here we report the preparation of prototype rigid/flexible encapsulated organic light-emitting electrochemical cells (OLECs), supported on ITO-coated glass and ITO-coated PET (Figure 1). The properties of the prototypical OLECs were characterized (i.e., voltage vs current curves as well as voltage vs emission power curves) and observed to operate as expected. The analysis of a combination of SDSs and *in silico* toxicity studies were used to assess the safety of the feedstocks used to produce the devices in line with "safe-by-design" principles, demonstrating this to be a useful method of minimizing potential environmental impacts from WEEE (exemplified with OLECs). This may be potentially useful in the development of future iterations of EEE in line with safe-by-design and safe and sustainable by design principles.[19]

Results and Discussion

OLEC Prototype Design and Characterisation

OLECs are one type of light-emitting devices with potential for a variety of technical and medical applications (e.g., large area light-emitting surfaces and devices for photobiomodulation), and their solution processable fabrication makes them attractive for industrial production.[20] The basic configuration and functional mechanism of LECs is illustrated in Figure S1. LECs consist of an ion- and electron-conducting blend as the active material which is sandwiched between the cathode and anode layer.[21a] Upon application of external bias, the ions in the active layer redistribute themselves and generate a p-doped region at the anode and n-doped region at the cathode. These p- and n-doped regions continue to grow with operating time, until they make contact and form a p-i-n junction. The exciton formed at the p-i-n junction causes light emission from conjugated polymers. Such dynamic formation of p-i-n doping structure brings the advantages that LECs, in contrast to OLEDs, can efficiently function independent to the work function of the electrodes and the thickness of the active material. Here we fabricated rigid and flexible OLECs supported on ITO-coated

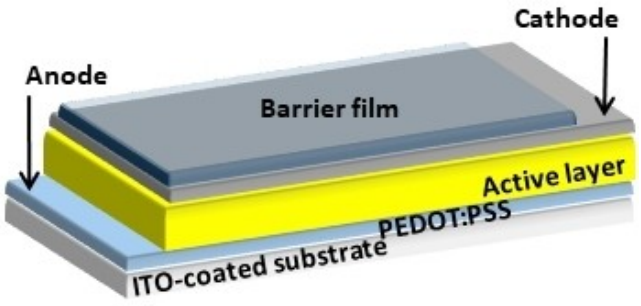

Figure 1. The layer-by layer structure of a LEC.

glass or ITO-coated PET, respectively, by spin-coating an anode and an active layer, followed by vapor deposition of a cathode. The transparent anode layer was composed of a conducting polymer poly(3,4-ethylenedioxythiophene) (PEDOT) and dopant poly(styrene sulfonate) (PSS), PEDOT:PSS;[21b] the active layer was composed of a mixture of Super Yellow, trimethylolpropane ethoxylate (TMPE-OH), and KCF_3SO_3;[21c,d] and the cathode was a vapor-deposited layer of Al. The design and manufacture process are depicted in Figures 1, S2 and S3. OLEC devices on rigid or flexible substrate (ITO-coated glass or ITO-coated PET, respectively) were investigated. The OLEC devices on ITO-coated glass and ITO-coated PET operated as expected, the I–V curves and the light emission OFF-/ON-states are shown in Figure 2. The OLECs on rigid or flexible substrates were functional and light-emitting, and stable device performance is achieved (Figure 3), clearly in the long term, device performance testing in combination with mechanical testing would be important to assess.

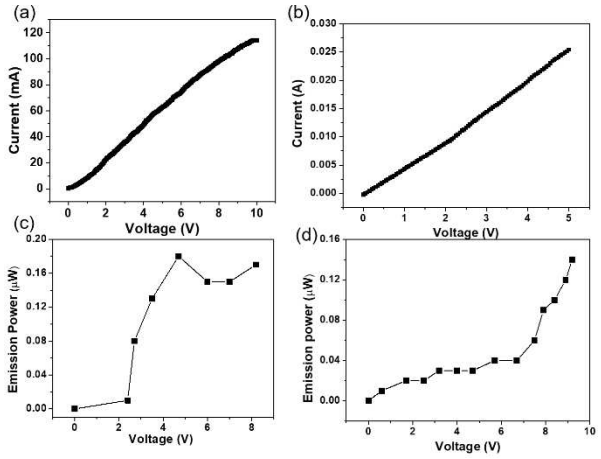

Figure 2. Optoelectronic analysis of the LECs. (a and b) Linear sweep voltammetry of the LECs on ITO-coated glass or ITO-coated PET, respectively. (c and d) Emission power of the LECs on ITO-coated glass or ITO-coated PET, respectively.

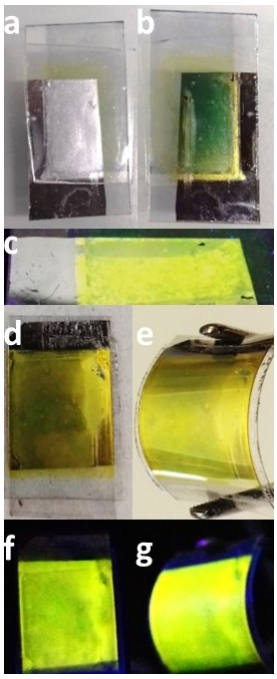

Figure 3. Images of the LECs on rigid and flexible substrates. (a and b) Photographs of ITO-coated glass supported LECs: (a) cathode up, and (b) cathode down). (c) Image of the ITO-coated glass supported LEC under UV light in the "ON" state. (d and e) Photographs of ITO-coated PET supported LECs: (d) cathode down flat, and (e) cathode down flexed. (g) Images of ITO-coated PET supported LECs under UV light in the "on" state: (f) flat, and (g) flexed.

OLEC Environmental and Health Considerations

WEEE presents a global challenge,[22] and the development of new technologies involves assessment of the hazards that substances used to produce and/or comprising the final product present to the environment and life.[23]

While aluminum, glass and PET (used in the cathode, rigid and flexible substrates, respectively) are widely recycled,[23c,d] that is reliant on sufficient quantities of each component being available for it to be economically viable, and profit-driven recycling markets result in recycling systems that do not necessarily produce the optimal environmental outcome.[23e]

Glass is generally recognized as safe by the U.S. Food and Drug Administration (FDA), likewise, PET is FDA compliant and food safe in both its virgin (unrecycled) state, and recycled state; however, Al (in the ionized state Al^{3+} state) is acknowledged to be toxic,[24] and the small amounts of Al present in the cathodes may not be economically viable to isolate/recycle meaning care would be necessary for disposal of devices into the environment,[25a] and suggesting alternative cathode materials may be better. The proprietary knowledge of the precise structure of the polymers/materials used to produce the KM barrier films, and the relatively small quantities of other components used in the production of these prototypical OLECs makes it challenging to understand how the prototypical OLECs might fit in a circular economy, particularly as these components may be viewed as contaminants of the aluminum, glass and/or PET used, complicating their route into a circular economy.[25b]

Computational approaches are applicable to safe-by-design and safe and sustainable by design principles approaches to product development, indeed, *in silico* toxicity screening methods have been primarily developed with the goal of designing high value small molecules (e.g., agrochemicals, medicines, etc.), thereby minimizing the number of in vivo tests undertaken to assess their safety, and safely facilitating product development.[26]

We have previously used a bioinformatics approach for *in silico* toxicity prediction in the development of electroactive materials for technical and medical applications,[27] specifically Derek Nexus to examine PEDOT, PSS and PEDOT-PSS (used in the anode coating) which were predicted to be non-sensitisers and non-mutagenic.[27e] Herein, we examined the risks associated with the other components used to produce the LECs in this study, using Derek Nexus (v.6.0.1) to assess the toxicity of the components found in the final prototype OLECs.

ITO (used to coat both the rigid and flexible substrates) is composed of indium oxide and tin oxide, that Derek Nexus examined as separate components, predicting that indium oxide is safe whereas tin oxide is plausibly a sensitizer (i.e., necessitating minimal exposure).[28] The SDSs for indium oxide and tin oxide highlight the UK Health and Safety Executive EH40/2005 workplace exposure limits for both to be of the order of mg/m^3 in powder form; listing the acute toxicity to rats (LD50) of tin dioxide to be $>$20 g/kg orally, and $>$2 mg/L via inhalation. The tin dioxide also shows toxicity towards: algae (No Observed Effect Concentration [NOEC] towards *Desmodesmus subspicatus* (green algae) to be 9.77 mg/L after 72 h, and the concentration of test substance which results in a 50% reduction in growth rate [ErC50] towards *D. subspicatus* (green algae) to be $>$100 mg/L after 72 h); bacteria (half maximal effective concentration [EC50] in activated sludge of $>$1 g/L after 3 h); daphnia magna (water flea) EC50 of $>$100 mg/L after 48 h; and fish (specifically *Oncorhynchus mykiss* [rainbow trout]) with a lethal concentration 50 (LC50, the amount of a substance suspended in the air required to kill 50% of test animals during a predetermined observation period) of $>$100 mg/L after 96 h.

The SDS for Super Yellow used in the active layer suggests it is not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008; and Derek Nexus predicts (based on examination of repeat units of Super Yellow) that it may display phototoxicity[29] and be a skin irritant.[30]

The SDS for KCF_3SO_3 used in the active layer highlights it to be an eye/skin irritant and to display respiratory toxicity; however, there are no alerts from Derek Nexus.

The SDS for TMPE-OH used in the active layer lists the acute toxicity to rats (LD50) to be $>$2 g/kg orally, and $>$2 g/kg via dermal exposure. The TMPE-OH also shows toxicity towards: algae with an EC50 towards *D. subspicatus* (green algae) of $>$100 mg/L after 72 h; bacteria with an EC50 in activated sludge of $>$1 g/L after 3 h; daphnia magna (water flea) with an EC50 of $>$100 mg/L after 48 h; and fish with a LC50 towards *Danio rerio* (zebra fish) of $>$1 g/L after 96 h; and Derek Nexus is equivocal if TMPE-OH displays nephrotoxicity.

The analysis of both the SDSs and *in silico* toxicity prediction data highlights that while the OLEC prototypes may be functional, there are opportunities for improvement regarding their design. It is noteworthy that the application of *in silico* toxicity prediction represents a valuable tool to developers of OLECs and other organic and flexible electronic products in academic and industry laboratories worldwide. Importantly, with health-related applications in mind, the results of *in silico* testing if encouraging (e.g., suggesting the materials are non-toxic, non-mutagenic, etc.) would de-risk the costs associated with ISO10993 studies that would be used to characterise the biocompatibility of the devices (& facilitate the eventual disposal of the OLECs at their end of life). Consequently, we believe that the impacts of this approach include short term impact via raising awareness of its potential utility and attitudinal openness to its use (highlighted herein), and long-term potential for economic, environmental, health and policy impacts.[30e]

OLEC Sustainability

Sustainable resource management is key to achieving the UN Sustainable Development Goals. We acknowledge that the life cycle assessment (LCA) for the prototypes described herein cannot be fully completed without having a system in place including known production and disposal routes, however, it is possible to make educated assessments of the 'sensitivity' of the different components. It is of key importance to know the 'functional unit', which is not per-device unless the device is single-use, this might be 'hours of illumination' in this case, 'number of patients treated' (for medical applications), or something else depending on the specific application, necessitating context-specific optimisation (e.g., low-impact for single-use devices; or long-life devices with multiple uses).[31a,b]

The glass-glass devices would have the longest life; however, recovery of the functional layers may be difficult if they are hermetically sealed into cell (e.g., via laser edge-sealing). The recycling route would be as per standard glass processing,[31c,d] noting that the organic materials would be combusted during the glass recycling process and the metallic elements would need to be extracted prior to this. For PET-PET devices, the PET can be recycled via either mechanical recycling (recovery & remelting or the thermoplastic polymer)[31e–g] or chemical recycling ('unzipping' of the polymer and subsequent extraction of the monomer and the other polymeric materials, including the adhesive layers and emissive materials).[31h,i] The removal and recovery of the metallic components would be through established methods (e.g., recovery of the metallic particles; dissolving the metals through a process such as a deep eutectic solvent, etc.).[31j–m] These options have pros and cons for either the cost of processing or the quality and reusability of the materials post-recovery (noting that new raw-materials may be lower cost than recycled materials, especially when additional processing or quality-checks are needed to ensure the quality of the materials is correct). For glass-PET devices there will be a relatively high carbon footprint because of the glass layer, but poorer barrier due to the PET layer and thus shorter device lifetimes. The recycling route at end-of-life would have to be to separate the PET and glass layers and then feed them into one of the routes described above, this could be achieved with an adhesive layer that is designed to fail at the right time (e.g., a heat seal). The final production route for these materials is likely to be a roll-to-roll process (for high throughput) rather than a batch process (for low volume bespoke products), and laminating barrier materials on either side may eliminate the need for the fluorinated components.

Generally, all products are well designed to be attractive to the end-user and to be manufacturable, and then depending on the economic model they may or may not be 'designed to be serviced' either by the end-user or by a qualified person. To meet the challenge of a regenerative and restorative society, a circular solution will need to 'design-for-X' to include design for re-use and design for materials-recovery at end-of-life. This will affect the design of the devices to include additional features that enable the parts to be efficiently identified and then separated for different recovery streams. Such features of these

LEC devices could be an adhesive layer that is designed to fail under exposure to unusual conditions (e.g., high temperature or a solvent), so that the layers can be separated for recovery. It is noteworthy that there are significant practical difficulties implementing circular economy which should not be underestimated, and for an overview of some of the complexities the avid reader is directed to an insightful article.[31n]

Conclusions

There are a multitude of approaches to prepare rigid and flexible light-emitting devices on various 2D and 3D substrates, and the development of flexible electronics is interesting as it offers opportunities for manufacturing next generation electronics (e.g., deformable devices, textiles, wearables, etc).[32] In principle OLECs can be prepared via solution processing, resulting in a light-emitting device capable of emitting various colours with a low driving voltage. We have demonstrated the capability to prepare encapsulated OLECs on both rigid and flexible substrates (specifically, ITO-coated glass and ITO-coated PET). While the preliminary performance results for the OLECs are promising, the results of our *in silico* toxicity prediction testing to assess the safety of the feedstocks used to produce the devices highlighted opportunities for improvement and the development of such devices in line with "safe-by-design" principles,[33] to minimize environmental impacts from OLEC-derived WEEE prior to scaling to industrial production. This approach to producing such technologies has many applications including opportunities for manufacturing next generation electronics such as deformable devices, smart textiles, wearables and diagnostics. Future research needs to address issues such as reduction in amounts of materials used to produce electronics, opportunities for reuse (e.g., increasing product lifetimes, repair paradigms) and for recycling (e.g., application of existing techniques to recycling electronic components, and addressing any issues with this, or developing new methods for recycling),[33c] and this should deliver better outcomes via the design and manufacture of electronics involving interdisciplinary teams of natural/materials/social scientists/engineers and people involved in various industry sectors.[34] It is also important to be aware of potentially disruptive innovations in the field including the emerging area of degradable/transient electronics.[35]

Experimental Section

Materials

Unless otherwise noted, chemicals were purchased from Sigma Aldrich (Gillingham, UK) and used as received. The glass vials and slides, micropipettes, plastic pipette tips, Parafilm®, hotplate stirrers and stir bars were supplied by Thermo Fisher Scientific (Morecambe, UK). Heat release Nitto Denko adhesive sheets (Nitto Denko UK Ltd, Mansfield, UK), and KM barrier film (KMB-002, KM Packaging Services Ltd., Peterborough, UK) were received as a gift from the Centre for Process Innovation (CPI, Sedgefield, UK). The Laurell Technologies WS-650 series spin coater (Laurell Technologies Corporation, Lansdale, PA, USA) was purchased from eBay. The materials were used to produce OLECs depicted in Figure 1, via the processes depicted in Figures S1, S2 and S3.

Cleaning ITO-Coated Glass/PET

The ITO-coated glass and ITO-coated PET were cut into square pieces with dimensions of 2 cm×2 cm using a diamond cutter. The square pieces of ITO-coated glass or ITO-coated PET were placed in a clean glass beaker containing soap solution and sonicated for 15 min at room temperature (25 °C). The liquid was discarded, replaced with fresh deionized (DI) water (≈10 mL) and sonicated for 10 min after which the liquid was discarded, (N.B. avoid over-sonication, as it may cause damage the ITO surface), then washed under a stream of DI water. Ethanol (≈5 mL) was added to the beaker, the ITO-coated substrates were sonicated for 10 min, and then the alcohol was discarded. Isopropanol (≈5 mL) was added to the beaker, the ITO-coated substrates were sonicated for 10 min, and then the alcohol was discarded. The beaker was covered with Al-foil perforated with a fine gauge needle, then placed in a vacuum oven at 80 °C for ≈2–3 h. Prior to use the slides were blown with a stream of N_2 gas.

Supporting ITO-Coated PET on Carrier Glass

A glass slide was cut to ≈2 cm×2 cm using a diamond cutter, rinsed with acetone and dried using a stream of N2 gas. The heat release Nitto Denko adhesive sheets were cut into squares with dimensions of 2 cm×2 cm, the thin interleave was removed and the adhesive sheet attached to the glass surface, after which the surface was gently rubbed using a lint free spatula to remove any air-bubbles. The cleaned and dried ITO-coated PETs were placed on a clean surface and the conducting side of the ITO-coated PETs was identified using a multimeter. The non-conductive side of the ITO-coated PETs were attached to the adhesive side of the heat release Nitto Denko adhesive sheet-coated glass substrates and any air bubbles removed by gently pressing the ITO surface using a lint free spatula, yielding glass slides with a heat release layer attached, and an ITO-coated PET substrate atop (ITO-coating facing up).

Coating the Anode Layer on ITO-Coated Glass/PET Substrates

Teflon tape (≈5 cm) was cut and wrapped tightly on one side of the ITO-coated glass or ITO-coated PET (the Teflon tape covered ≈2–3 mm of the surface of the ITO-coated substrate), after which the substrates were placed in a UV ozone cleaner (PSDP Pro Series Digital UV-Ozone Cleaner, PSDP UV4T, Novascan, Ames, Iowa, USA) at 60 °C for 20 min.

To 300 μL of ethanol was added 100 μL of PEDOT:PSS solution (1.1 % in H_2O, surfactant-free, high-conductivity grade); the mixture was sonicated at room temperature for 30 min to ensure its homogeneity after which it was checked to ensure there are no big particles of PEDOT:PSS left in the mixture.

The ITO-coated substrates were removed from the UV ozone cleaner (PSDP Pro Series Digital UV-Ozone Cleaner, PSDP UV4T, Novascan, Ames, Iowa, USA) and placed on the rotating disk of the spin coater Laurell Technologies WS-650 series). PEDOT:PSS mixture (100 μL) was dropped on the ITO-coated substrates, and spin coated at 500 rpm for 10 s, then 2000 rpm for 1 min, after which they were transferred to a vacuum oven at 80 °C for 3–4 h. The PEDOT:PSS layer is the anode layer of the device.

Transmittance of PEDOT:PSS coated ITO-glass/PET was measured using an Agilent spectrophotometer, optimizing the spin coating process to ensure the transmittance was suitable to use over the range 380–700 nm (>70% transmittance). The thickness of the PEDOT:PSS layer was ≈100 nm as determined using a profilometer (KLA-Tencor Alpha-Step® IQ, KLA Corporation, Milpitas, CA, USA).

Coating the Active Layer Blend on the Anode Coated Substrates

8 mg of Super Yellow (SY, a polyphenylene-vinylene (PPV) material) was dissolved in 1 mL of cyclohexanone by stirring at room temperature for 24 h. 25 mg of trimethylolpropane ethoxylate (TMPE-OH, Mn≈450) was dissolved in cyclohexanone (1 mL) and the mixture stirred at room temperature for 24 h. KCF_3SO_3 was dried overnight in vacuum oven at 100 °C. 10 mg of vacuum dried KCF_3SO_3 was dissolved in cyclohexanone (1 mL) and the mixture stirred at room temperature for 24 h. The active layer blend was prepared by mixing SY:TMPE-OH:KCF_3SO_3 in 1:0.15:0.03 solute mass ratios. This was obtained by mixing 1 mL of SY solution, 48 μL of TMPE-OH solution and 24 μL of KCF_3SO_3 solution together at room temperature for 12 c to obtain at homogeneous mixture. Teflon tape (≈5 cm) was cut and wrapped tightly on one side of the ITO-coated substrate (the Teflon tape covered ≈2–3 mm of the surface of the ITO-coated substrate), after which the substrates were placed on the rotating disk of the spin coater (Laurell Technologies WS-650 series). 100 μL of active layer blend was deposited on the centre of the ITO-coated substrates and spin coated at 500 rpm for 10 s, then 2000 rpm for 1 min; this active layer coating was repeated via the same procedure three times to ensure a uniform coating, and the substrates were placed in a vacuum oven at 80 °C overnight. Al films were deposited on substrates at room temperature (MiniLab 060, Moorfield Nanotechnology Limited, Knutsford, Cheshire, UK). The thickness of the active layer was ≈1 μm and the thickness of the Al cathode layer was ≈100 nm, as determined using a profilometer (KLA-Tencor Alpha-Step® IQ, KLA Corporation, Milpitas, CA, USA).

Coating the LECs with Barrier Films

ITO-coated glass and glass-supported ITO-coated PET LECs were stored under N_2 in a glove box (Omega model, Saffron Scientific Equipment Ltd., Knaresborough, North Yorkshire, UK) to avoid contact with moisture and air until the point at which they were used. The KM barrier film (KMB-002) and poly(butylene succinate) (used as a protective film) were cut in a shape shown in Figure S3. The encapsulation process was undertaken in an atmosphere of N_2 to minimize/prevent air being trapped in the sealed devices which will diminish performance due to a certain amount of oxidation of the top electrode and decomposition of the active layer.

For ITO-coated glass LECs, the protective film was removed from the barrier film, and the barrier side will be attached to the surface of the LEC (air/N_2 bubbles were removed by gently pressing the surface using a lint free spatula). The materials were stored overnight in a vacuum oven at 50 °C, after which they were transferred to a glove box (Omega model, Saffron Scientific Equipment Ltd., Knaresborough, North Yorkshire, UK) for storage.

For glass-supported ITO-coated PET LECs with a Nitto Denko adhesive sheet were stored under N_2 in a glove box (Omega model, Saffron Scientific Equipment Ltd., Knaresborough, North Yorkshire, UK) to avoid contact with moisture and air until the point at which they were used. They were transferred to the surface of a hotplate kept in the glove box at 100 °C. The glass support was in contact with the hotplate for ≈2–3 min until the heat release Nitto Denko adhesive sheets lost their tackiness allowing detachment of the LEC from the carrier glass using forceps. The KM barrier film (KMB-002) and poly(butylene succinate) protective film were cut in a shape shown in Figure S3. The protective film was removed from the barrier film, and the barrier side will be attached to the surface of the LEC (air/N_2 bubbles were removed by gently pressing the surface using a lint free spatula). The materials were stored overnight in a vacuum oven at 50 °C, after which they were transferred to the glove box for storage.

Optoelectronic Analysis of LECs

LECs were placed inside a dark chamber. The photodiode from Thorlabs was fixed 3 cm above the LEC and connected to a computer and controlled by ThorLab software. The LEC was connected to a potentiostat controlled by Ivium software, via crocodile clips (the red WE was connect to the Al-cathode, the blue RE and black CE were connected together and connected to the PEDOT:PSS anode). The dark chamber was closed and the photodiode switched on (ThorLab software confirming 0 power), the potentiostat was turned on and connected via the Ivium software. Standard linear sweep voltammetry was selected, and the following settings were input (E start = 0 V, E end = 10 V, E step = 10 mV, scan rate = 101 mV/s). Auto current range (AutoCR) was chosen to measure I–V curves. The change in emission power (as detected by the photodiode) with time was recorded and voltage vs current curves as well as voltage vs emission power curves were plotted.

In Silico Toxicity Studies

In silico toxicity screening studies of the polymers was carried out using Derek Nexus (v.6.0.1, certified knowledge base 2018 1.1) in Nexus v.2.2.2 provided by Lhasa Ltd. The simplified molecular-input line-entry system (SMILES) notations were entered into the integrated structure editor in Nexus and default prediction settings were used for Derek Nexus. Any compound activating an alert with a reasoning level of "equivocal" or above was treated as a positive prediction from the system. The SMILES notations for the components studied herein are listed hereafter in parentheses (): indium oxide ([In](O[In] =O) =O), tin dioxide ([Sn](=O)=O), KCF_3SO_3 (S(C(F)(F)F)(O)(=O)=O), TMPE–OH (C(COCCO)(COCCO)(COCCO)CC) and Super Yellow (C1(=C(C=C(C(=C1)OCCCCCCCCCC)C=CC2=CC=C-C(C(=C2)C3=CC=C(C=C3)OCCCCCCCCCC)C=CC4=CC=C(C-=C4)C5=CC(=CC=C5)OCCCCCCCCCC)C=CC)OCCCCCCCCCC)C).

Supporting Information Summary

The supporting information includes. Figure S1. Basic configuration and functional mechanism of LECs. (a) Configuration of LECs. Schematic representation of LEC operation (b) before and (c) under an applied forward bias. (d) The recombination of injected electrons and holes in emissive layer caused by the redistribution of anions and cations. Figure S2. The process used to prepare the LECs. Figure S3. LEC preparation. (a) Schematic showing the shape of the KM barrier film that is attached to LECs. (b) Example photographs of the front and back view of the LECs.

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Conflict of Interests

The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, or in the decision to publish the results.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords: Conjugated polymer · Light-emitting electrochemical cell · Light-weight and flexible device architectures · Solution-based fabrication · Materials science

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