Metal-Containing Functional Materials for OLEDs and Solar Cells

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I. Introduction

II. Organic Light-Emitting Devices (OLEDs)

III. Electrophosphorescent OLEDs

IV. Organic Photovoltaics (OPVs)

V. Metal-based Materials for Solar Cells

VI. Conclusions and Future Prospects
Energy Interconversions

Photovoltaic Cells (Solar Cells):
*Electricity from Light (Sunlight)*

Organic Light-Emitting Diodes (OLEDs):
*Light from electricity*
History of Light

Thomas Alva Edison (1847-1931)
Light is a form of energy

To create light, another form of energy must be supplied. The two common ways are *incandescence* and *luminescence*.
Incandescence refers to the emission of light from heat energy.

e.g. An electric stove’s heater or metal in a flame glows “red hot”

The tungsten filament of an ordinary incandescent light bulb glows “white hot”
The Sun and stars

Direct sunlight  5400 K
100 W Tungsten bulb 2865 K
Candle flame  1930 K
Luminescence

• *Luminescence* refers to the emission of light from other sources of energy, which can take place at normal and lower temperatures. It is commonly termed “*cold light*” emission

• Several types of luminescence can be distinguished depending on the excitation source
## Different Forms of Luminescence

<table>
<thead>
<tr>
<th>Luminescence type</th>
<th>Excitation Source</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Catholuminescence</td>
<td>Electrons</td>
<td>TV sets, monitors</td>
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<tr>
<td>Photoluminescence</td>
<td>(UV) Photons</td>
<td>Fluorescent lamps, plasma displays</td>
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<tr>
<td>Chemiluminescence</td>
<td>Chemical energy</td>
<td>Lightsticks, environmental analysis</td>
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<td>Bioluminescence</td>
<td>Biochemical energy</td>
<td>Analytical chemistry, maintenance of life</td>
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<td>Electroluminescence</td>
<td>Electric field</td>
<td>LEDs, EL displays</td>
</tr>
<tr>
<td>Triboluminescence</td>
<td>Mechanical energy</td>
<td>—</td>
</tr>
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</table>
Photoluminescence (PL)

- The emission of light triggered by absorption of photons

\[ h\nu \rightarrow A^* \rightarrow h\nu' \lessgtr h\nu \]

Absorption (Excitation) \hspace{3cm} Emission

A* (excited state)
Fluorescent liquids
Lighting and Electricity

• Lighting consumes about 30% of all electricity used in a building.
• In USA, that translates into 18% of the total energy being used in a building.
• In HK, the highest energy consumer is air-conditioning. The next highest is lighting. This is especially true in commercial buildings.
• This trend is expected to permeate and propagate into mainland.
Lighting accounts for 19% of all Electrical Energy Used World-wide
• Incandescent light is still responsible for about 40% of all the lighting.
• Its power efficiency is 12-17 lm/W.
• Solid state light sources (LEDs or OLEDs) can easily be 4-5 times higher.
• For OLED, laboratory demonstration of 30-60 lm/W has been achieved.
Electroluminescence (EL)

• The emission of light by electric current

• Historical development
  a. 1962 (Holonyak and Bevacqua)
    • Inorganic semiconductors for light-emitting diodes (LEDs)
      e.g. p-n junction diodes
    • The energy of the light emitted can be changed by adjusting the composition of the material
Electroluminescence (EL)

- $p$-type semiconductors: the added material has fewer electrons than the host and adds positive holes e.g. Si doped with B
- $n$-type semiconductors: the added material has one more electrons in the valence shell than the host material e.g. Si doped with As
Electroluminescence (EL)

- Crystal of pure silicon
- Silicon doped with arsenic (n-type)
- Silicon doped with boron (p-type)
Electroluminescence (EL)

Device structure for common LEDs

Crystal substrate (transparent)

$n$-type

$p$-type

Light output

+ 

−
1987 (Tang and VanSlyke in Kodak)

- Fluorescent organic dyes as electroluminescent materials for organic light-emitting devices (OLEDs)
1990 (Richard Friend in Cambridge University)
- Luminescent conjugated polymers for polymer light-emitting devices (PLEDs)
  e.g. poly(1,4-phenylene vinylene) (PPV) is a famous light-emitting polymer

PPV
Features of OLEDs

- Self-emitting property
- High luminous efficiency
- Full color capability
- Wide viewing angle
- High contrast, low power consumption, low weight
- Large-area color displays and flexibility
Basic Principle of OLEDs

(a) Small molecules and polymers

(b) OLED structure:
- Cathode
- Organic emitter
- Anode
- Substrate
Theory of OLEDs or PLEDs

• The simplest OLED or PLED configuration consists of an electroluminescent layer sandwiched between an anode and a cathode, one of which has to be semi-transparent

• Under an applied bias, injection of holes takes place at the anode whereas injection of electrons occurs at the cathode
Some of the electrons and holes combine within the emissive material to form singlet (25%) and triplet excited states (75%). Such an electron-hole pair (exciton) may then result in the emission of a photon.
Theory of OLEDs or PLEDs

- Unfortunately, the mobility of electrons and holes in most organic materials are considerably different, leading to exciton formation in the vicinity of one of the two contacts (For example, since holes migrate much more easily through PPV than electrons, electron-hole recombination takes place near the cathode)
• Since non-radiative exciton recombination, or quenching, is enhanced at the electrode-organic interface, the single-layer structure typically exhibits a low quantum efficiency
⇒ Heterojunction OLEDs
Layers in OLEDs

- **Hole-Transporting Layer (HTL)**
  - Transports holes from the anode to the EML or ETL
- **Electron-Transporting Layer (ETL)**
  - Transports electrons from the metal cathode to the EML or HTL
• **Emission Layer (EML)**
  – Transports both holes and electrons
  – The layer where the recombination of holes and electrons takes place

Double layer membrane

Either ETL or HTL behaves as EML
Layers in OLEDs

Triple-layer device

The recombination of holes and electrons occurs in an independent EML.
Common Layer Materials in OLEDs

HTL materials e.g. PPV, TPD, NPD

TPD

α-NPD
ETL materials, e.g. PBD, Alq$_3$

Oxadiazoles are electron-deficient
Polymers have bigger molecules and therefore cannot be thermally deposited.

Instead, thin films are spin coated onto the substrate.

Although it has advantage of fabricating device in ambient atmosphere, it has solvent problem when depositing multi-layer thin films.
Fluorescence vs Phosphorescence

Energy level diagram for a photoluminescence system

- Absorption
- Internal Conversion
- Intersystem Crossing
- Fluorescence 25%
- Phosphorescence 75%
Iridium(III) Complexes

- One of the best phosphorescent dyes at present
- Effective intersystem crossing by spin-orbit coupling
- High phosphorescence efficiency at room temperature
Literature examples for color tuning

red shift of emissions
[Ir(ppy-X)₂(acac)] with main group elements

Ir-SO₂

Ir-S

Ir-O

Ir-N

Ir-PO

Ir-Ge

Ir-Si

Ir-B
Multi-color OLEDs at 8 V

Sunlight Duplicator

White Organic Light-emitting Devices

CIE (0.354, 0.360)  CRI = 97
Activate spot: 6.25 cm² @ 8V
Two-Color WOLEDs

Maximum efficiencies

\[ \eta_L = 42.9 \text{ cd/A} \]
\[ \eta_P = 20.3 \text{ lm/W} \]
\[ \eta_{\text{ext}} = 19.1\% \]
Efficient White Polymer Light-emitting Devices for Solid-State Lighting

ITO Emission layer (70-80 nm) Ba (4 nm) PEDOT:PSS (40 nm) Al (100 nm)

SO\textsubscript{3}HS O\textsubscript{3}SO\textsubscript{3}HS O\textsubscript{3}SO\textsubscript{3}H

PEDOT:PSS

WOLEDs vs Incandescent/Fluorescent Bulbs
The goals of developing renewable energy sources can only be achieved by solutions from the chemical sciences in all steps.

**Photovoltaic Cells (Solar Cells):** Electricity from Sunlight

**Solar Energy:** The Clean Energy for the 21st Century
Why solar energy?

Solar energy: renewable, environmentally friendly, abundant and free
Solar Spectrum

US Dept. of Energy

Image: NREL
Renewable Energy vs Fossil Fuels

• **Fossil fuels** including coal, oil, and natural gas provide more than 90% of the energy consumed in a modern society.

• **Fuels** are substances that when burned release significant amounts of energy together with CO$_2$ emission. Fuels are not unlimited.
Harvesting Solar Energy

• Harnessing the Sun: **Solar Energy**
  It has been noted that nearly all of the energy available on Earth comes from the Sun.
• Energy from the Sun is diffuse and must be concentrated to make it useful.
• Chemistry can develop more efficient materials for photovoltaics to transform sunlight into electricity.
Primary Energy Use in The World

(PVNET-European Roadmap for PV R&D, JRC-EUR21087 EN, 2004)
Photovoltaics-Projections

Figure 2. Cumulative Net Clean Energy Payoff

Source: NREL
Photovoltaic cells (solar cells) can be used to convert solar energy into electricity. These devices can be made from a variety of substances e.g. elemental Si, light-absorbing dyes, organic semiconductors (small-molecules or polymers).
Biomass: Photosynthesis for Fuel

Burning plant material by-products is one means of harvesting energy from the Sun.

Water \( (H_2O) \) is split to produce Oxygen \( (O_2) \) and Carbon Dioxide \( (CO_2) \). The electrons from this reaction are used to convert Water into Sugar. 

Natural Photosynthesis: The Solar Cell Model
Inorganic Semiconductor (Silicon) Solar Cell

Individual cell

Modules
• **Advantages**
  – Lifetime- 15-20 years for systems, up to 30 years for modules
  – No pollution, no waste products
  – Energy from the Sun is free and abundant
  – It is cleaner, safer, and renewable

• **Disadvantages**
  – High initial cost (although it is recovered by fuel savings over the lifetime of the product)
  – Area intensive (can be solved by utilizing roofs and surfaces in urban areas, deserts etc.)
  – Intermittence and seasonality of sunlight – need for storage of energy
Applications

• Solar cells are useful in a wide range of applications.
  – Space
  – Solar cell modules in calculators and wrist watches
  – one of the key technologies towards a sustainable energy supply.
Steckborn, Switzerland.
First church in the world with solar power
Organic solar cells

• Advantages
  – Low cost
  – Large area
  – Flexible substrates and devices
  – Improved coverage of solar spectrum

• Disadvantages
  – Low efficiency
  – Low exciton diffusion length
  – Low charge carrier mobility
  – Inferior stability compared to inorganic materials
Why organic solar cells?

Flexible photovoltaic diodes

Silicon solar cell (left) and plastic film solar cell (right)
Schematic representation of flexible and easy produce organic materials

Polymer photovoltaic cells with flexible substrate
Dye-sensitized solar cells (DSSCs)

A schematic diagram of the energy flow in the dye-sensitized solar cell

Dye

electrolyte

TiO₂

counter electrode

electrically conductive glass electrode

sunlight

3 I

I₃⁻
Dye-sensitized solar cells (DSSCs)

- The ruthenium-based dye collects incident light – in the same way as green chlorophyll molecules harvest sunlight in plants.
- The dye is absorbed onto the surface of a semiconducting electrode of TiO$_2$. Once excited by light, the dye molecules lose electrons and are oxidized by TiO$_2$. They are then reduced by iodide ions present in the electrolyte solution.
- The resulting iodine produced is then itself reduced at a second electrode to complete the cycle.
- The electrons injected into TiO$_2$ travel around the external circuit and do the work for the user.
- Relatively high efficiency (> 10%), cheap, extremely promising as clean energy sources.
Bulk Heterojunction Solar cells

Glass substrate
Anode (ITO)
PEDOT:PSS
Metallopolyyne:PCBM
Cathode (Al)
Current-Voltage Curve of Solar Cell

\[ J_{\text{sc}} = \text{short-circuit current} \]
\[ V_{\text{oc}} = \text{open-circuit voltage} \]
\[ FF = \text{fill factor} \]
\[ \eta = \text{power conversion efficiency} \]
Research on Conjugated Organic Polymers
Optimum photovoltaic performance for some reported organic polymers

<table>
<thead>
<tr>
<th>Polymer</th>
<th>$E_g$ [eV]</th>
<th>$E_{\text{HOMO}}$ [eV]</th>
<th>$E_{\text{LUMO}}$ [eV]</th>
<th>$V_{\text{oc}}$ [V]</th>
<th>$J_{\text{sc}}$ [mA cm$^{-2}$]</th>
<th>FF</th>
<th>PCE [%]</th>
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<td>0.55</td>
<td>5.50</td>
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</table>
• Synthesis of low bandgap organic polymers
• New electron-acceptors
• Exploitation of tandem solar cells using multiple layers of different bandgaps

• *Any alternative?* ⇒ Organometallic polymers
Organometallic Photovoltaics

Literature reports:

• Dye-sensitized solar cells using small-molecule organometallic donor materials (Grätzel-type cell)

• Organic solar cells based on metal phthalocyanines
Typical solar cell structure

Small molecule OPVs

Fullerene ($C_{60}$)

Metal Phthalocyanine
Research on Metallopolyynes

- Good solution-processibility
- Excellent model systems to study the photophysics of excited states in conjugated polymers
- Effective intersystem crossing into triplet state due to the *heavy atom effect* (harvesting of triplet state energy)
Research on Metallopolyynes

Transition Series

- Variation of metal centers (M)
- Variation of spacer groups (R)
- Variation of auxiliary ligands (L)
Applications in Optoelectronics and Nanotechnology

Metallopolyynes

Luminescence
PLEDs
Nanomaterials
Optical limiting
Photovoltaics/Solar Cells
Liquid Crystals and Chemosensing
Cover page, Hot article
太陽能電池可薄如保鮮紙

太陽能電池能否如保鮮紙，又薄又能捲曲？今年裏德基金會「優秀科研獎」得獎者之一、浸會大學化學系教授黃維揚，利用有機金屬聚合物，成功研發聚合物太陽能電池。全球首次以有機金屬製成的太陽能電池。

仍未到40歲的黃維揚笑說：「未來的太陽能電池有可能薄如一張保鮮紙。」他指出，有機金屬聚合物太陽能電池的最高能量轉換效率僅達4%，惟傳統無機半導體太陽能電池的逾10%為高，但已經處於國際領先水平。

將製大面積捲曲顯示器

他的研究又將與染料應用於高效及穩定的多色及白光有機發光二極管（LED）等新產品，成本低、低能耗的全彩色顯示器及室內照明系統，「日後將可製成大面積且可捲曲的顯示器，有助廣告商宣傳」。

黃維揚：創新金屬材料 助研太陽能電池

一些金屬物質加入有機聚合物中，形成另一種新型材料。從60年代開始研究，發現新材料可吸收更多可見光區的太陽光，理論上具很大潛力提高器件中電流的轉換及遷移率，令電池更高效及耐用。目前新材料用在太陽能電池上，其最高能量轉換效率為4%，遠遠低於國際及消費者水平。黃維揚指，「根據研究理論，這類材料的最高效率可進一步提升至10%。他希望在未來5年進一步提升新材料的性能，將效率提高至7%到8%。」

新產品成本低效率高

黃維揚表示，新型太陽能電池相比傳統的無機半導體太陽能電池，除效能更高外，未來的製造過程也可更簡化，成本更低，重量更輕。有別於傳統的柔軟型，未來更可製造出不同形狀，覆蓋面積更大的柔性電池或電池模。另外，黃維揚亦有意將其重點於硝化染料電池的研究。相關材料對新一代的全彩色顯示技術，及室內照明系統的發展都有重要意義。
Metallopolyynes as New Functional Materials for Photovoltaic and Solar Cell Applications

Light Conversion to Electricity

- Absorption of photon, leading to the formation of an exciton (bound electron-hole pair)
- Exciton diffusion to a region where exciton dissociation (charge separation) occurs
- Charge transport of electrons and holes within the layer to the respective electrodes
- The resulting photocurrent and photovoltage can charge a battery
Current Status

- MP1
- MP2
- MP3
- MP4
- MP5
- MP6
- MP7
- MP8
- MP9
- MP10
- MP11
- MP12
- MP13
- MP14
- MP15
- MP16
Physical data and photovoltaic performance of **MP6-MP16** /PCBM (1:4) best devices

<table>
<thead>
<tr>
<th>Polymer</th>
<th>$E_g$ [eV]</th>
<th>$E_{\text{HOMO}}$ [eV]</th>
<th>$E_{\text{LUMO}}$ [eV]</th>
<th>$V_{oc}$ [V]</th>
<th>$J_{sc}$ [mA cm$^{-2}$]</th>
<th>FF</th>
<th>PCE [%]</th>
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<tr>
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<td>-5.37</td>
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<td>0.81 (0.90)$^b$</td>
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<td>0.36 (0.63)$^b$</td>
</tr>
</tbody>
</table>

a) Optical bandgaps determined from the onset of absorption in solid state.
b) At Pt polyyne/PCBM (1:5, w/w) ratio.
Comparison of the optical data of various low-bandgap platinum(II)-based metallopolyynes with different spacer Ar.

![Chemical structure](image)

<table>
<thead>
<tr>
<th>Ar =</th>
<th>Color</th>
<th>Maximum $\lambda_{\text{max}}$ in solid film / nm</th>
<th>$E_g$ / eV</th>
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<tbody>
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<td>446</td>
<td>2.55</td>
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<td><img src="image" alt="Chemical structure" /></td>
<td>Orange-red</td>
<td>528</td>
<td>2.20</td>
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<td><img src="image" alt="Chemical structure" /></td>
<td>Purple</td>
<td>548</td>
<td>1.85</td>
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<td><img src="image" alt="Chemical structure" /></td>
<td>Deep blue</td>
<td>650</td>
<td>1.77</td>
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<td><img src="image" alt="Chemical structure" /></td>
<td>Deep green</td>
<td>681 (R = H) 714 (R = C\textsubscript{6}H\textsubscript{13})</td>
<td>1.50 (R = H) 1.47 (R = C\textsubscript{6}H\textsubscript{13})</td>
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<tr>
<td><img src="image" alt="Chemical structure" /></td>
<td>Deep blue-green</td>
<td>660</td>
<td>1.58</td>
</tr>
</tbody>
</table>
Metallated conjugated polymers as a new avenue towards high-efficiency polymer solar cells

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Donor-Acceptor Concept

Dark purple 1.85 eV

Yellow 2.55 eV

Orange yellow 2.20 eV
Absorption and Photophysics

Strong absorption in the visible region
**Photovoltaic Behavior**

![Graph showing the photovoltaic behavior of MP6 and P3HT, with absorbance and EQE plots.](image)

**Absorbance (a.u.):**

- MP6:PCBM
- P3HT:PCBM

**EQE (%):**

- MP6
- P3HT

**Voltage (V):**

- MP6
- P3HT

**Wavelength (nm):**

- MP6:PCBM
- P3HT:PCBM
Phase separation occurs for films with a 1:4 blend ratio, whereas films with a 1:1 ratio are smooth.
Factors Influencing the Nanometer-scale Morphology of Polymer Blends

- The solvent (affecting the drying time during film formation)
- The relative blend ratio between polymer and electron acceptor
- The polymer solution concentration
- The primary chemical and electronic structures of the metallopolyynes
Hole and electron mobilities in MP6:PCBM blends
Effects of Metalation

• Extending the absorption to longer wavelengths without the need of triplet excitons
• Involvement of triplet excitons in the high-efficiency energy conversion
• Enhancing conductivity and mobility?
• Affecting the structural features and packing arrangement?
Tuning of Polymer Solar Cell Efficiency
Absorption and Photophysics

$J$-$V$ curves of solar cells with MP7-MP10:PCBM (1:4) active layers under simulated AM1.5 solar irradiation
Effect of blend composition on solar cell performance

MP9:PCBM

MP10:PCBM

P3HT:PCBM
Hole and electron mobilities in MP7-MP10:PCBM blends

\[ \mu_h (\text{cm}^2 \text{V}^{-1} \text{s}^{-1}) \]

\[ \mu_e (\text{cm}^2 \text{V}^{-1} \text{s}^{-1}) \]

\[ E^{1/2} (\text{V}^{1/2} \text{cm}^{-1/2}) \]

\[ E^{1/2} (\text{V}^{1/2} \text{cm}^{-1/2}) \]
Effect of Oligothienyl Chain Length on Tuning the Solar Cell Performance in Fluorene-Based Polyplatinynes

Absorption spectra in CH$_2$Cl$_2$ at 293 K

$J-V$ curves of solar cells with MP11-MP14:PCBM (1:5) active layers under simulated AM1.5 solar irradiation

The comparison between hole ($\mu_h$) and electron ($\mu_e$) mobilities in MP11-MP14:PCBM blends obtained by the SCLC modeling
Polymer solar cells based on very narrow-bandgap polyplatinynes with photocurrent extended to the near-infrared (NIR) region

UV-Vis absorption spectra
MP3  $E_g = 2.55$ eV
MP5  $E_g = 1.77$ eV
MP16  $E_g = 1.47$ eV
Organometallic photovoltaics shed new light on the road to commercial polymer solar cells to solve the energy crisis.
To become more widely used, the production cost of modules must be reduced.

Due to relatively large investment costs, government incentives are important. The biggest users of solar energy: US, Europe, Japan.

Developing technologies for thin film and organic solar cells may enable production of inexpensive and efficient modules.

This area sheds light on the road to commercial polymer solar cells to solve the energy crisis.

Projected target is efficiency (>5%), lifetime (>3 years) and cost (<US$0.5/Wp). Currently, there is no commercial OPV yet.
Challenges in Organometallic Research – Great Opportunity for OLEDs and Solar Cells

- Organometallic molecules have become a field of intense activities in the optoelectronic research. They hold great promise as versatile functional materials for use in energy interconversions.
Alternately, new and environmentally more friendly light sources are being introduced.

The development of these light sources required new materials, devices and fabrication conditions.

These new light sources allow us to design new types of lamp that can revolutionize illumination.
The End
Thank You!