R&D Project Management in the Chemical Industry

The following collection of PowerPoint® Charts is intended to further clarify and supplement the relevant specialist publications on the subject matters dealt with. This collection in no way is used for any commercial purposes, but as learning material for students.

Selected sources for in-depth studies of the respective subject matters are given in some lists of references.

The chemical-technical target components listed in the case study tasks, the formulas, deadlines, economic and technical data as well as the data in the "profile boxes" are widely with a practical orientation, but purely fictitious.

They are solely used for a vivid depiction of the methods and as exercise materials.

Congruence with the target sets of third parties would be coincidental.

Rainer Buerstinghaus

R&D Project Management
in the Chemical Industry

Supplementary Module 03 for Chemists (m/f/d)

Information Material *for the subject matter:*
Cathodic Electrodeposition Paints/Coatings.

"Electrodeposition Coatings for the Corrosion Protection of Car Bodies."

Rainer Buerstinghaus

R&D Project Management in the Chemical Industry

Subject Matter

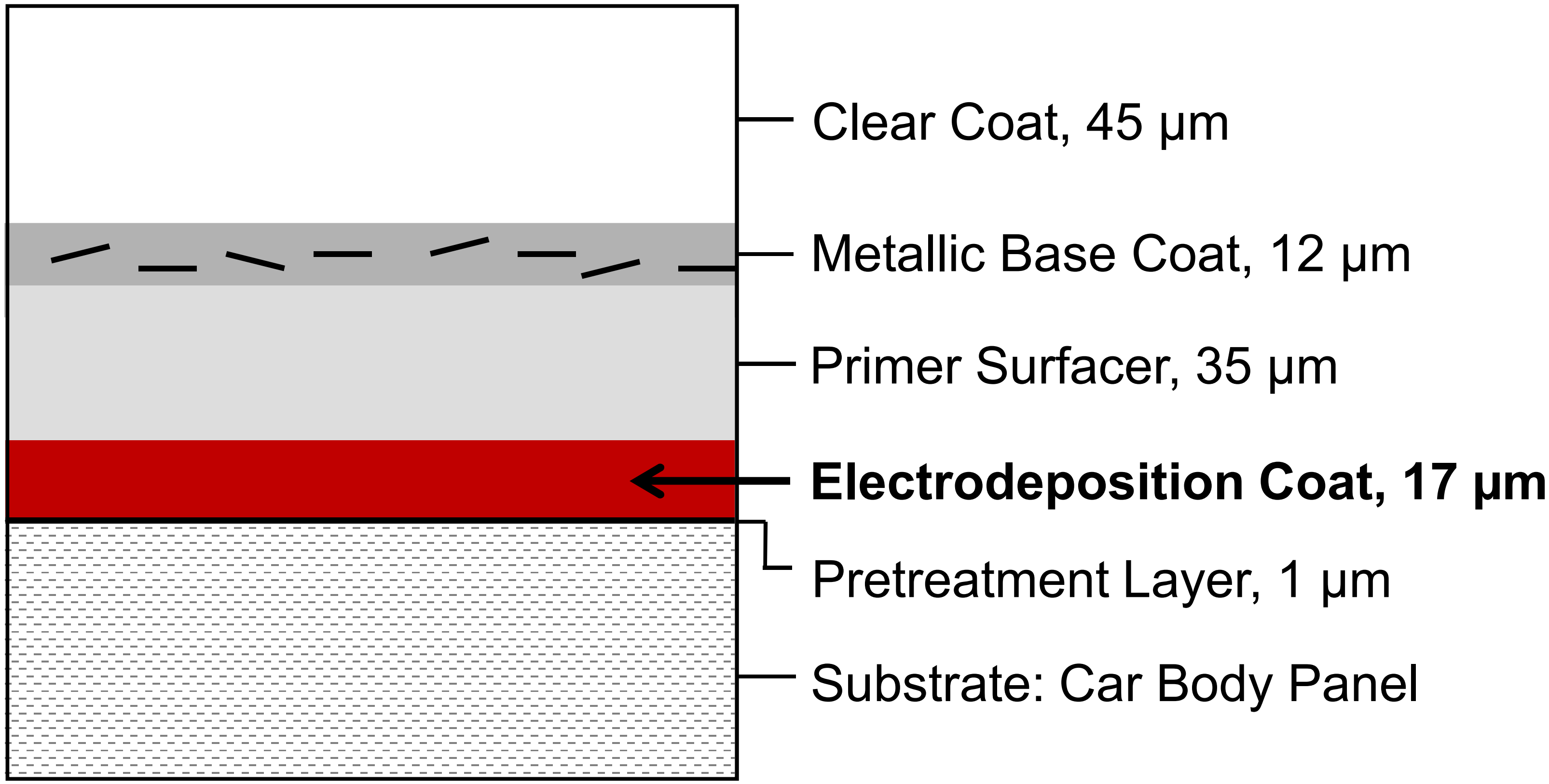
Cathodic Electrodeposition Paints/Coatings.

Chemical-Technical Basics:
"Electrodeposition Coatings for the Corrosion Protection of Car Bodies."

Rainer Buerstinghaus

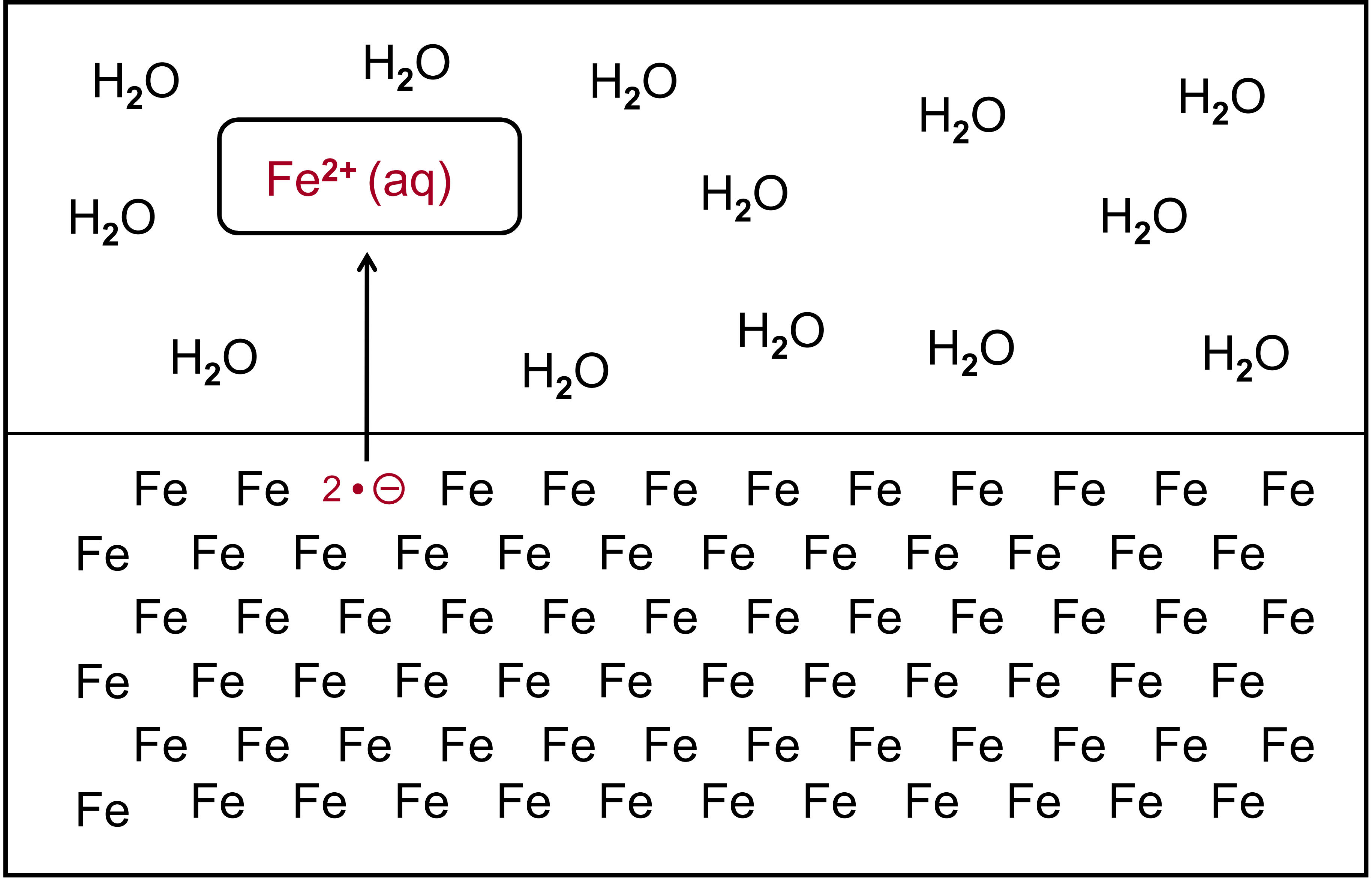
Four-Layer Automotive Painting, 2020

Typical Layer-Structure, Standard Technology (OEM).



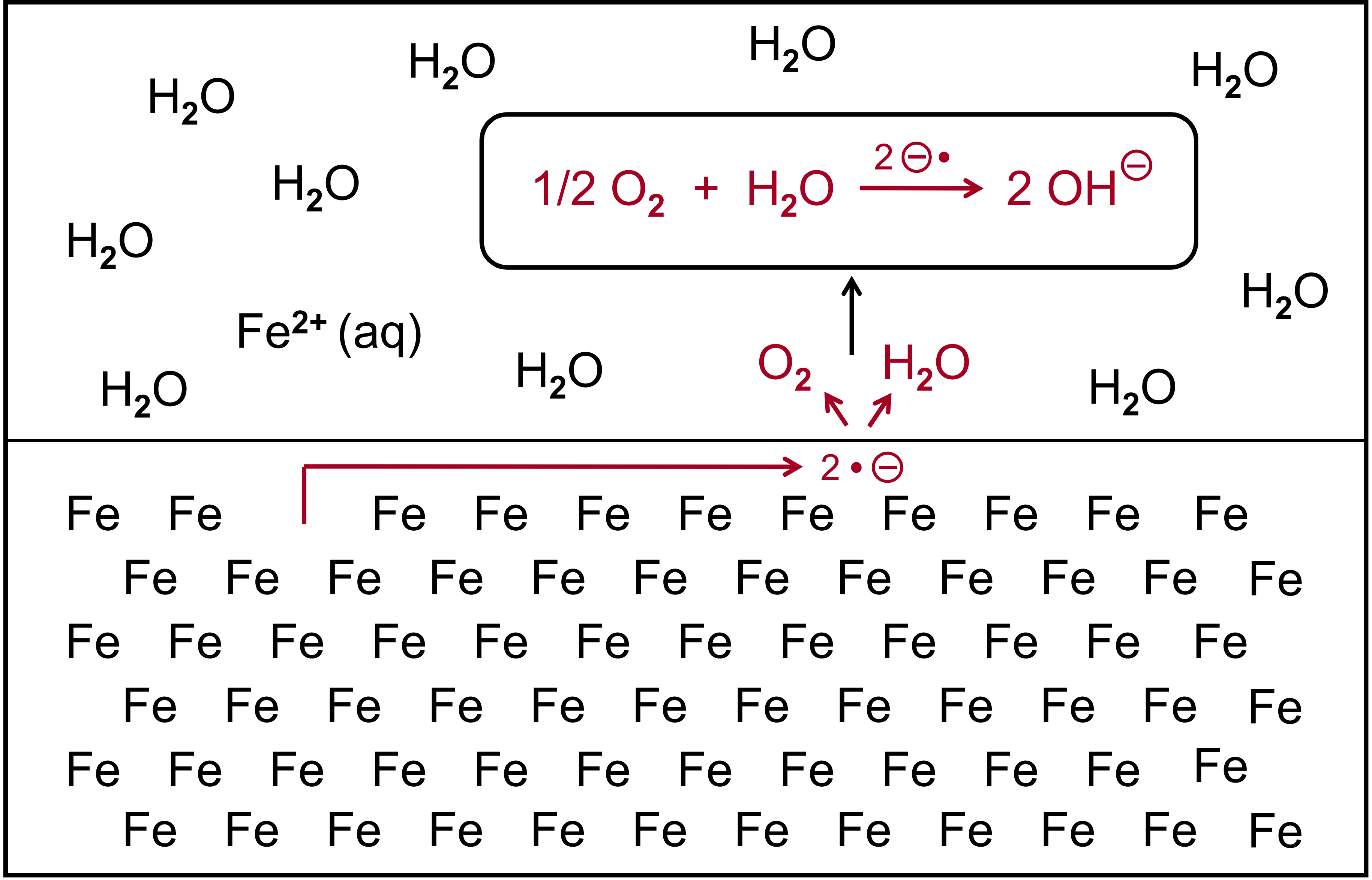
Rainer Buerstinghaus

Electrodeposition Coatings for the Corrosion Protection of Car Bodies: Corrosion Process: **Anodic Reaction**.



Rainer Buerstinghaus

Electrodeposition Coatings for the Corrosion Protection of Car Bodies: Corrosion Process: **Cathodic Reaction**.



Rainer Buerstinghaus

Electrodeposition Coatings for the Corrosion Protection of Car Bodies: Corrosion Process: **Individual Steps**.

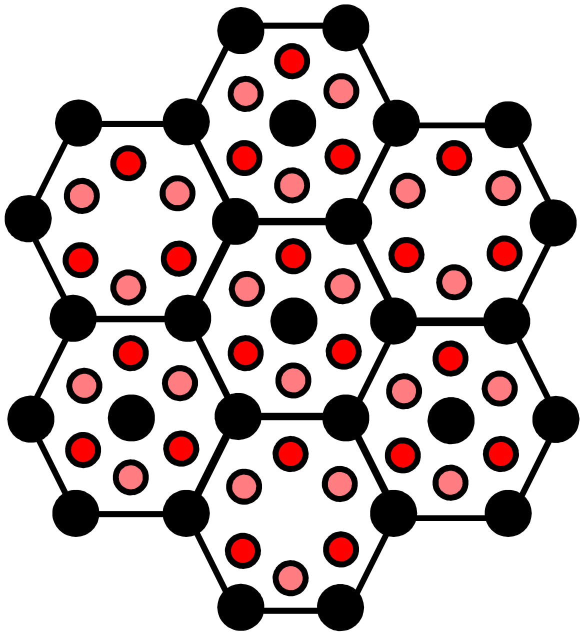
$Fe \xrightarrow{-2 \bullet \ominus} Fe^{2+}$
$H_2O + ½\, O_2 \xrightarrow{+2 \bullet \ominus} 2\, OH^{\ominus}$
$Fe(OH)_2 \longrightarrow FeO + H_2O$
$2\, Fe(OH)_2 \xrightarrow[+ H_2O]{+ ½\, O_2} 2\, Fe(OH)_3$
$2\, Fe(OH)_3 \xrightarrow[- 2\, H_2O]{} 2\, FeO(OH) \xrightarrow[- H_2O]{} Fe_2O_3$ (Hematite)

Rust: $x\, FeO \cdot y\, Fe_2O_3 \cdot z\, H_2O$	(x, y, z: Independently from each other: 1, 2, 3, 4, …)

Rainer Buerstinghaus

Coating of Phosphated Steel with Epoxy Resins

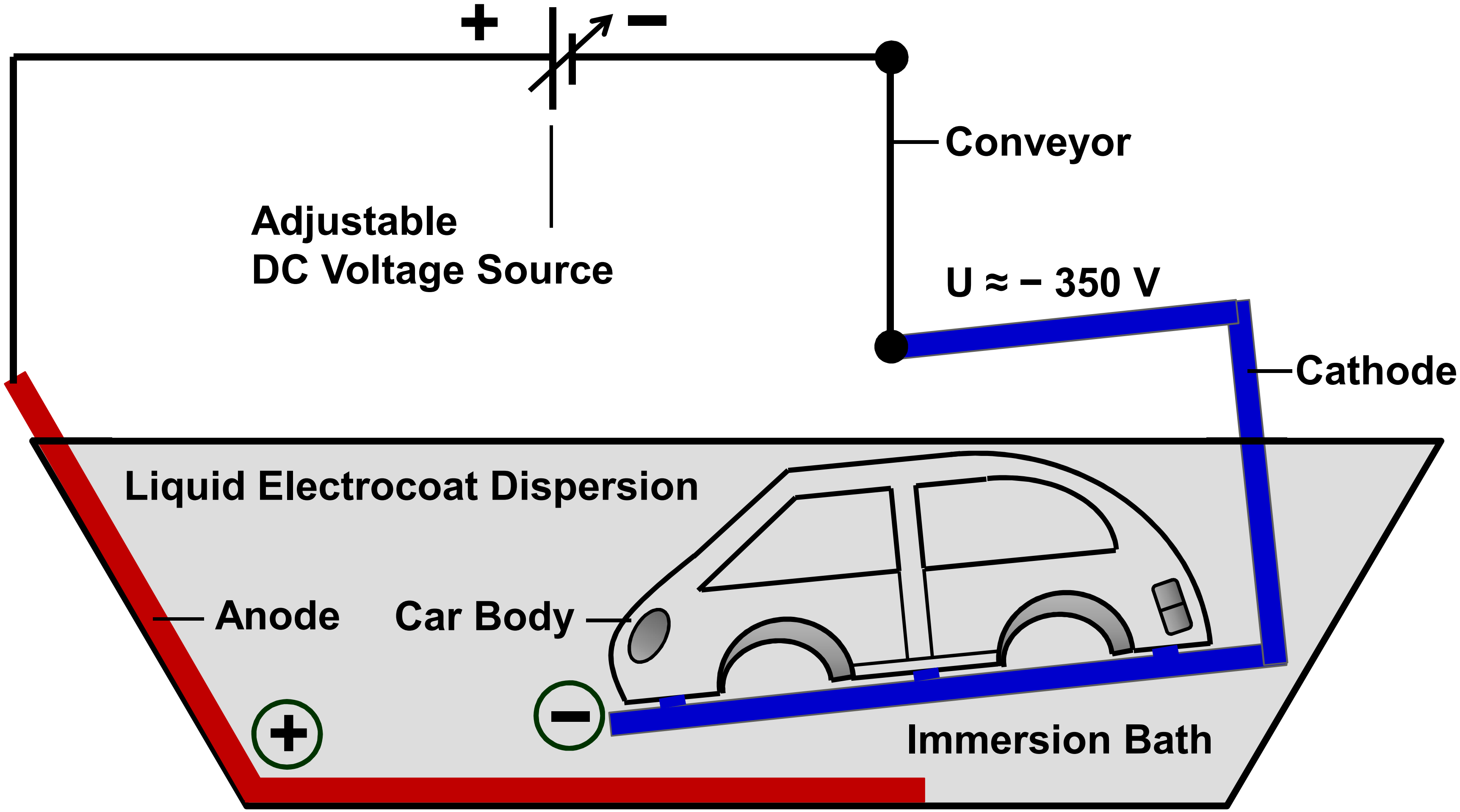
Fe_2O_3 - Structural Detail in Vertical Projection.



	28X ● (Fe^{3+})
	42X ● bzw. ● (O^{2-}) ("Different Altitudes")
	28 : **2** = 14 14 X **3** = 42
("Corundum Structure", Detail)	→ **(Fe^{3+}) / (O^{2-}) = 2 / 3**

Rainer Buerstinghaus

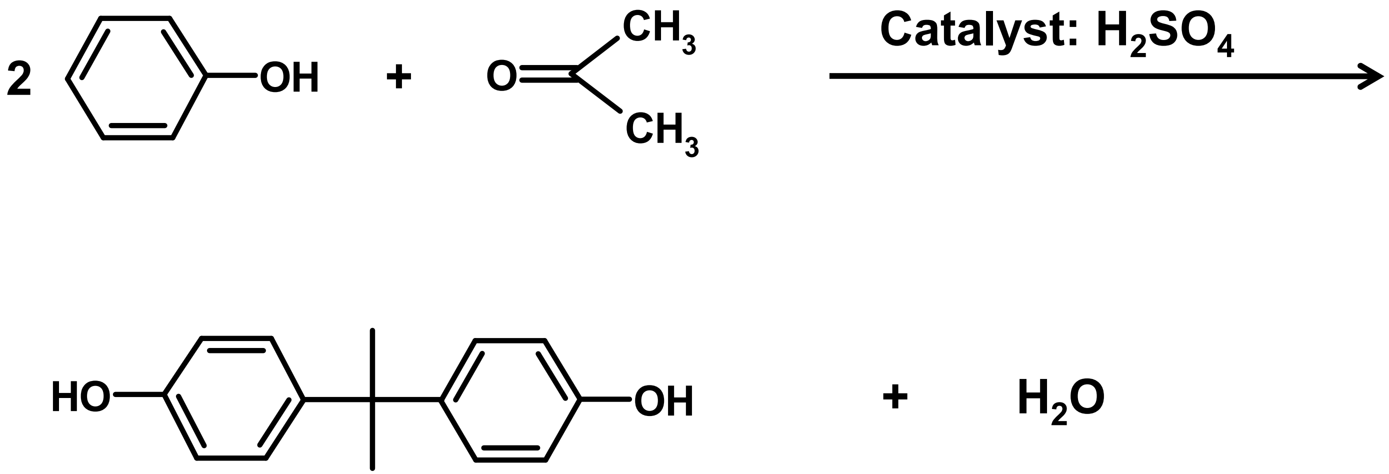
Electrodeposition Coatings for the Corrosion Protection of Car Bodies: Cathodic Deposition Process: Principle.



Rainer Buerstinghaus

Coating of Phosphated Iron with Epoxy Resins.

Bisphenol-A, Technical Synthesis from Acetone and Phenol.

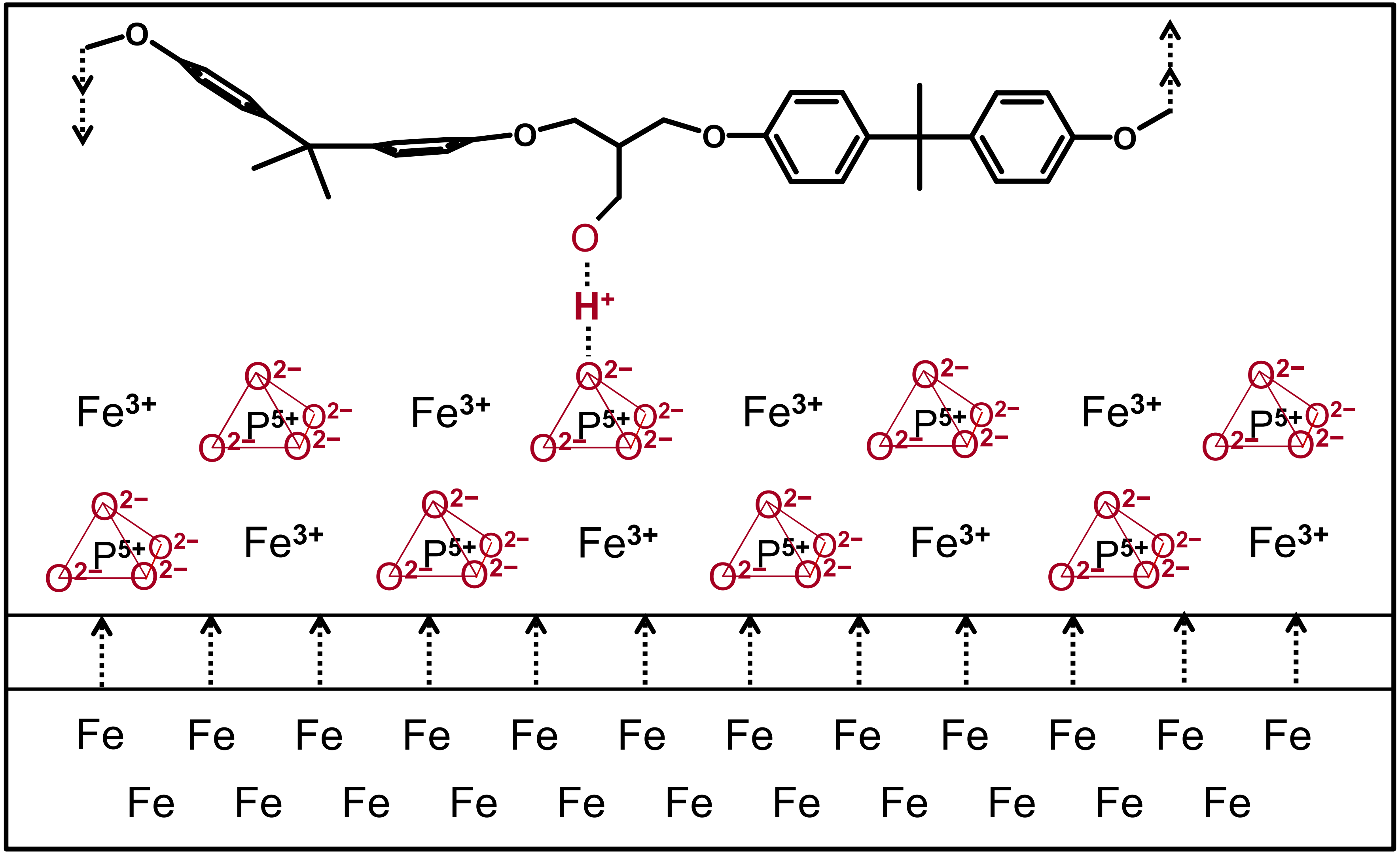


Alternative Catalysts: HCl-Gas + CH_3SH (Hooker-Process) Acidic Ion Exchangers (UCC-Process).

Rainer Buerstinghaus

Coating of Phosphated Iron with Epoxy Resins.

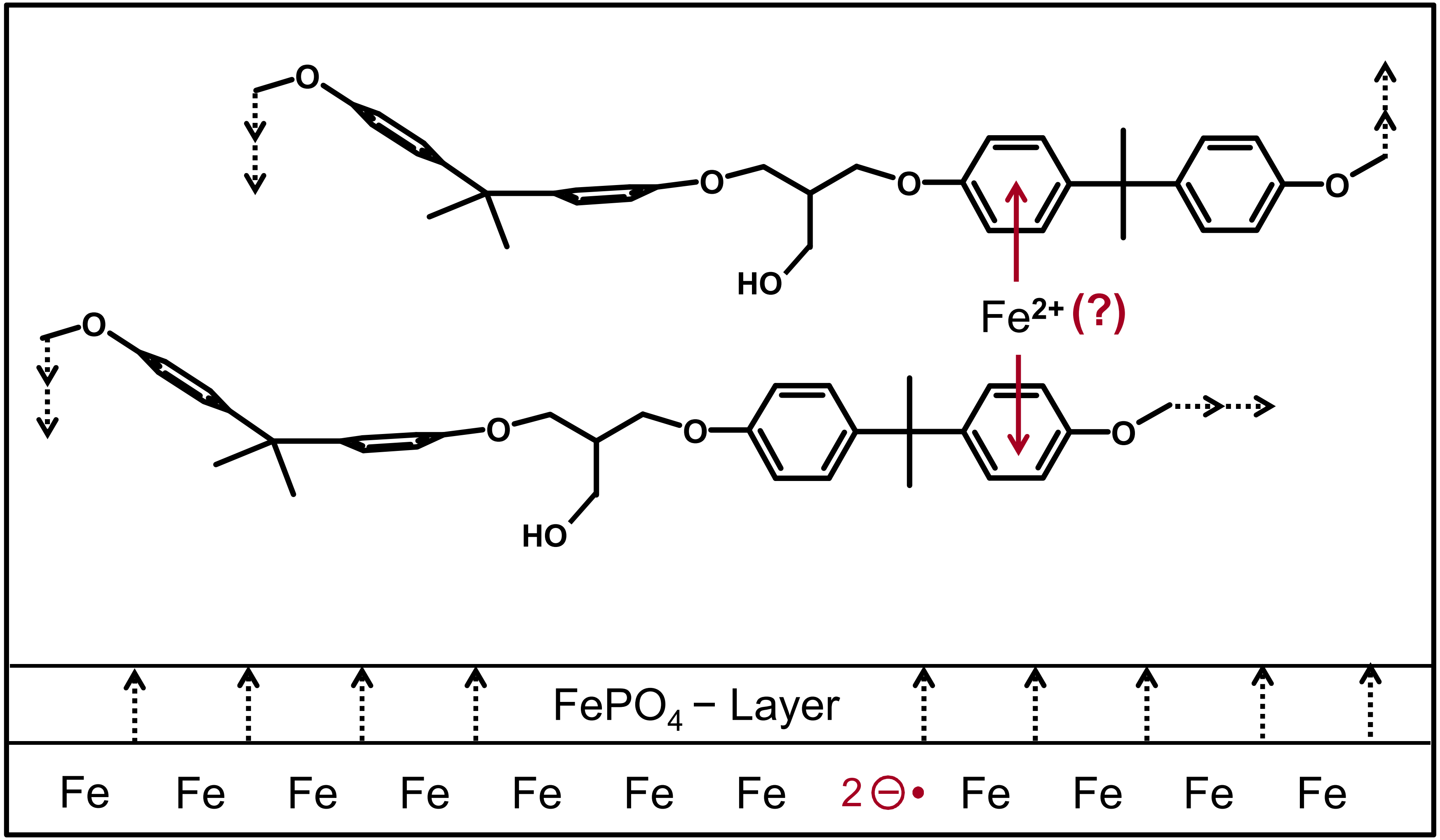
Corrosion Protection: Adhesion to the Surface through H^+–Bridges.



Rainer Bürstinghaus

Coating of Phosphated Iron with Epoxy Resins.

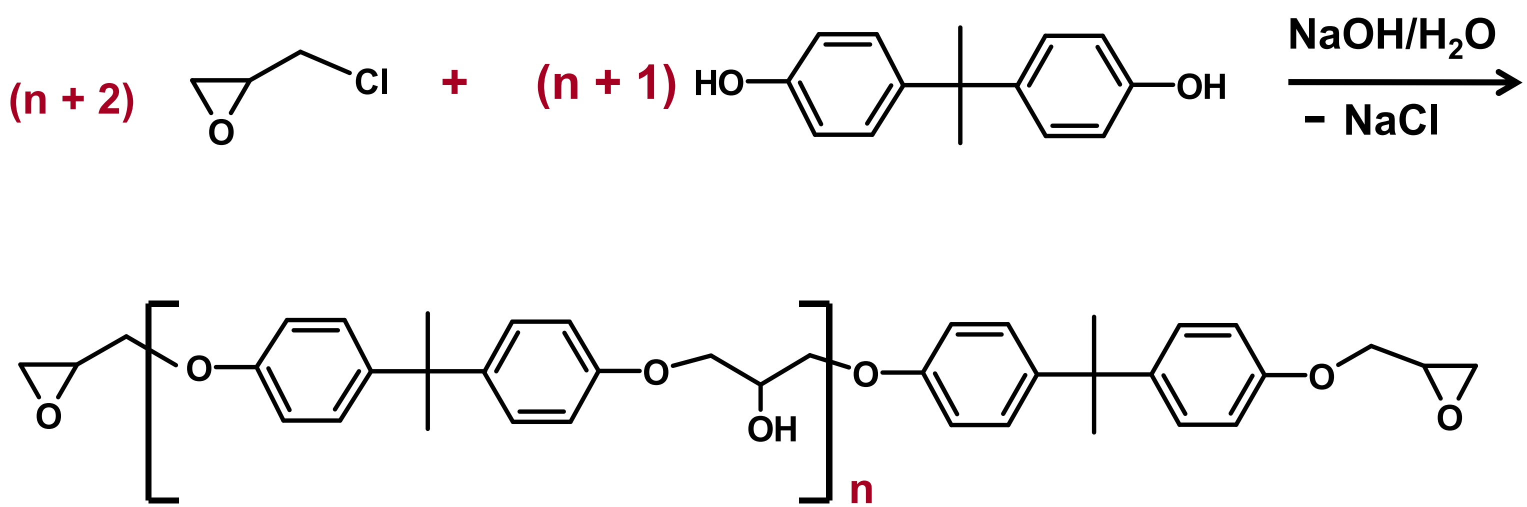
Corrosion Protection: Complexation of "Free" Fe^{2+}- Ions between Electron Rich, Aromatic Rings (?) (Idealized Representation).



Rainer Buerstinghaus

Coating of Phosphated Iron with Epoxy Resins.

Epoxy Resin Synthesis from Bisphenol-A and Epichlorohydrin.
Control of the Molecular Weight Distribution via Molar Number n.

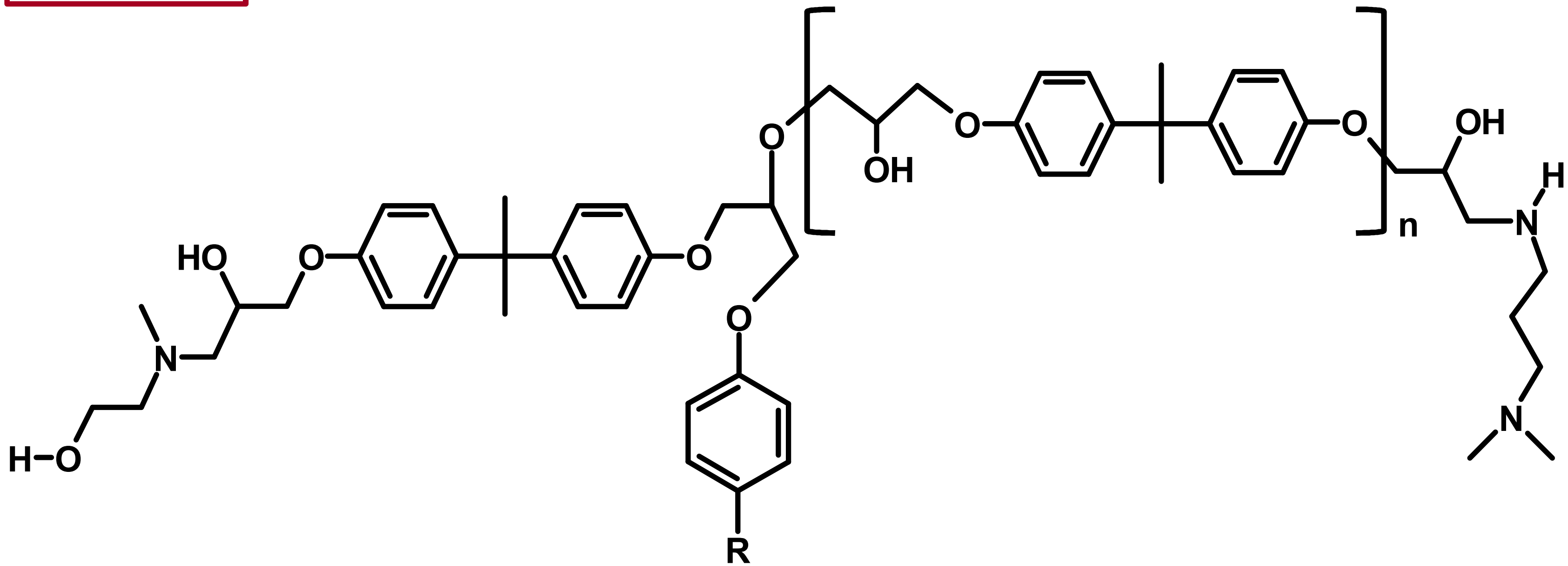


n = 0,1,2,3,…..29,30...

Rainer Buerstinghaus

Electrodeposition Coatings for the Corrosion Protection of Car Bodies: CED Basic Resin (Simplified Representation).

Example



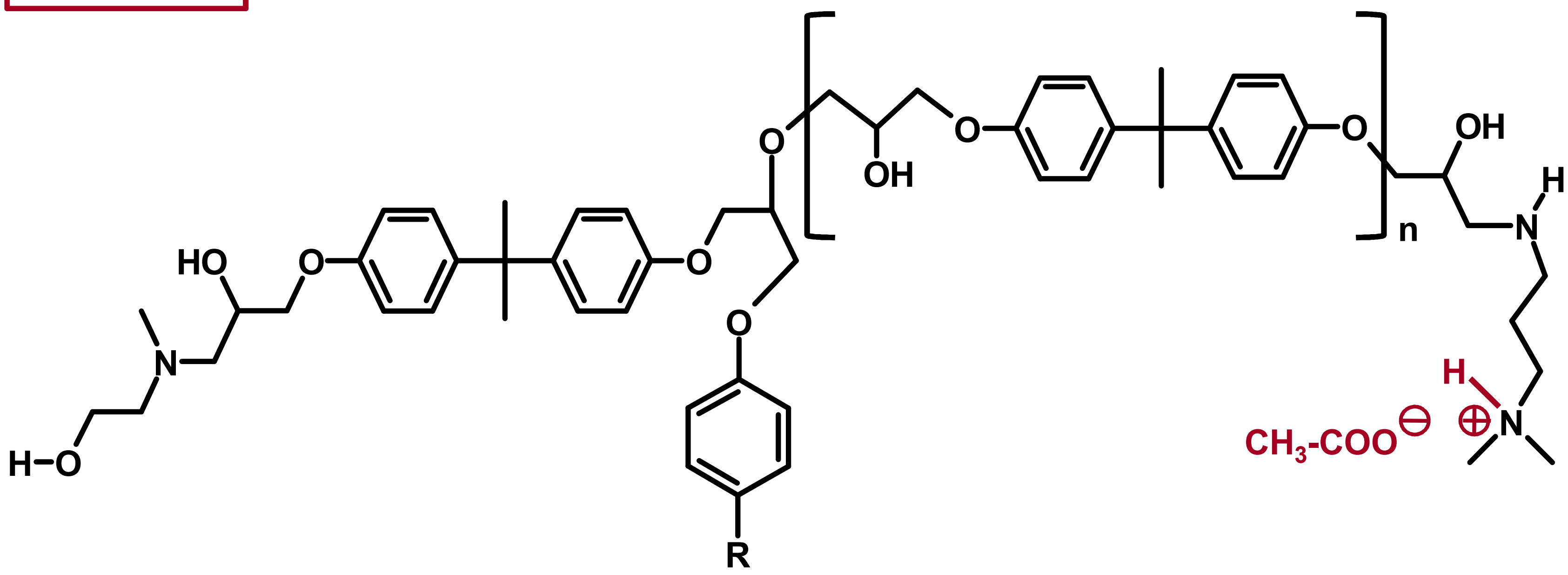
R = CH_3 (75%-100%); n-$C_{12}H_{25}$ (0%-25%) n = 3,4,5,…

After addition of acetic acid or lactic acid, the amine-modified epoxy resin forms the corresponding ammonium compound: →

Rainer Buerstinghaus

Electrodeposition Coatings for the Corrosion Protection of Car Bodies: CED Basic Resin (Simplified Representation).

Example

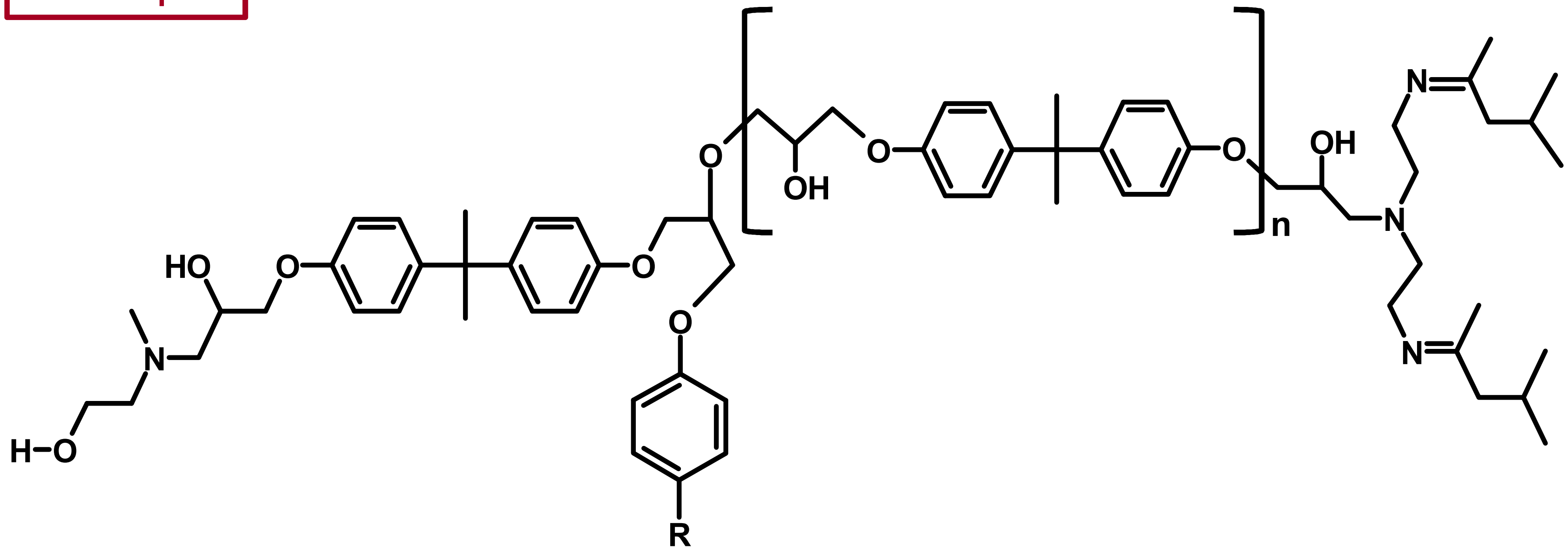


R = CH_3 (75%-100%); n-$C_{12}H_{25}$ (0%-25%) n = 3,4,5,…

The protonated, amine-modified epoxy resin forms a stable, electrophoretically depositable secondary dispersion in water.

Electrodeposition Coatings for the Corrosion Protection of Car Bodies: CED Basic Resin (Simplified Representation).

Example



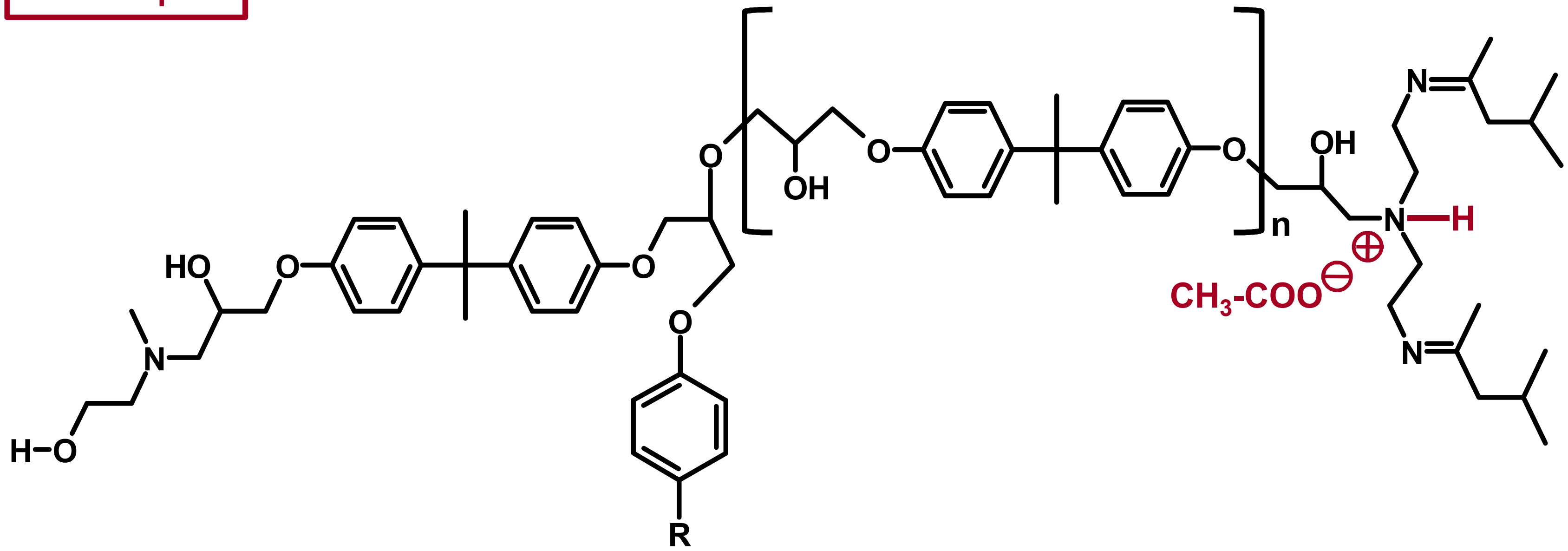
R = CH_3 (75%-100%); n-$C_{12}H_{25}$ (0%-25%) **n = 3,4,5,…**

After addition of acetic acid or lactic acid, the amine-modified epoxy resin forms the corresponding ammonium compound: →

Rainer Buerstinghaus

Electrodeposition Coatings for the Corrosion Protection of Car Bodies: CED Basic Resin (Simplified Representation).

Example



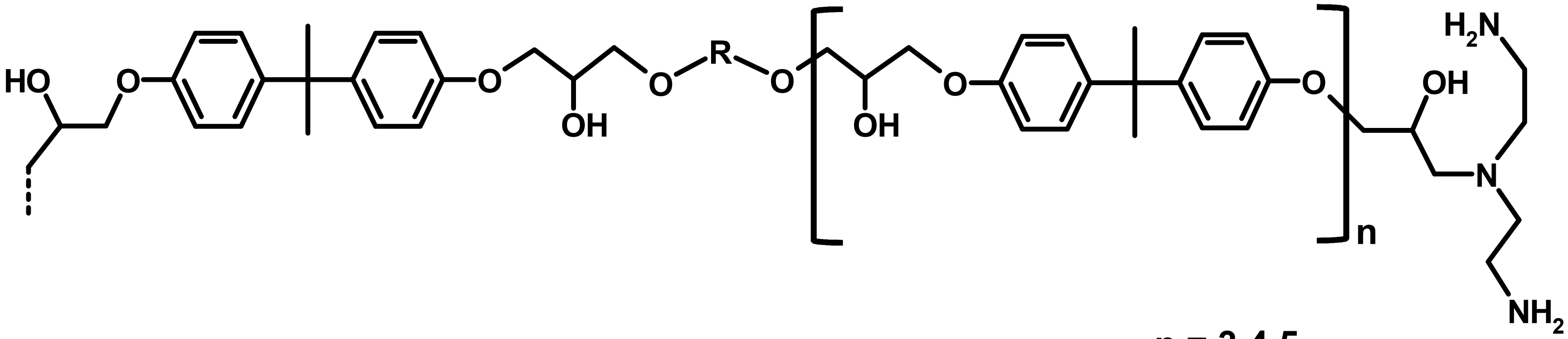
R = CH_3 (75%-100%); n-$C_{12}H_{25}$ (0%-25%) n = 3,4,5,…

The protonated, amine-modified epoxy resin forms a stable, electrophoretically depositable secondary dispersion in water.

Rainer Buerstinghaus

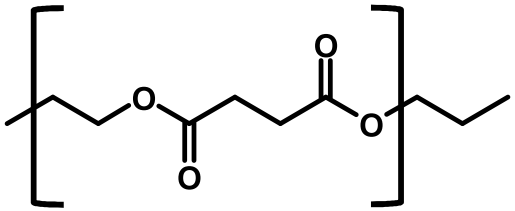
Electrodeposition Coatings for the Corrosion Protection of Car Bodies: CED Basic Resin (Simplified Representation).

Example

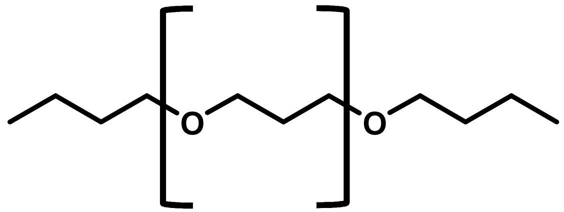


n = 3,4,5,…

–R– = e. g. :



m = 2, 3,4,5,…



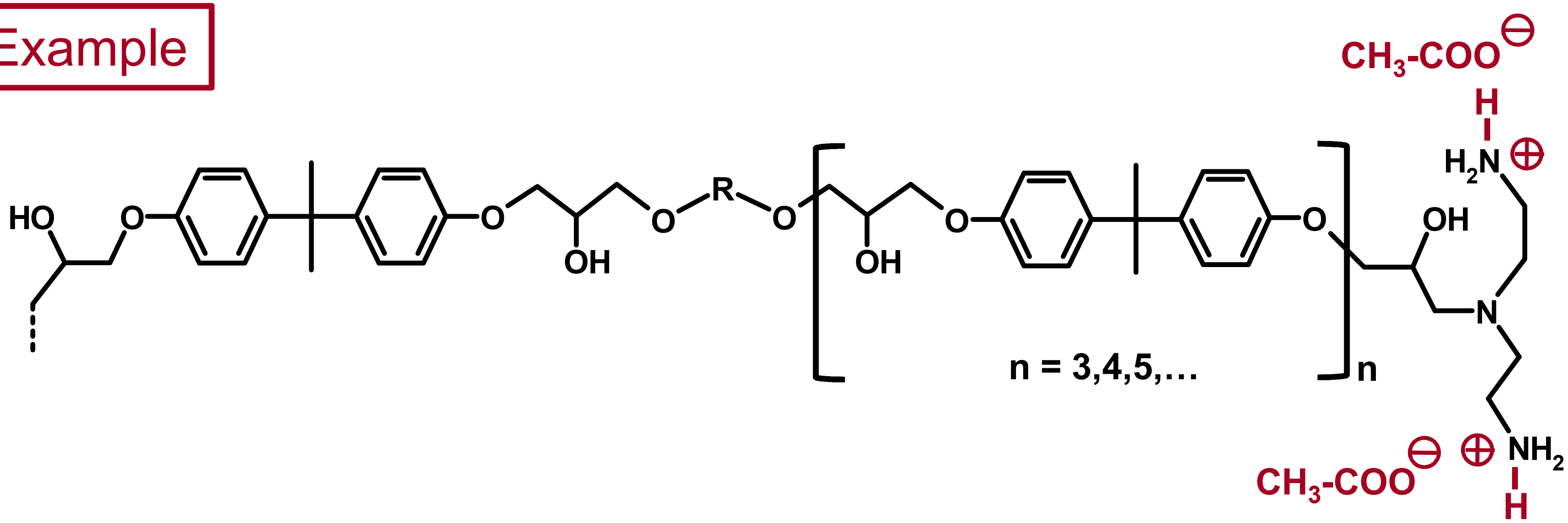
l = 2, 3,4,5,…

After addition of acetic acid or lactic acid, the amine-modified epoxy resin forms the corresponding ammonium compound: →

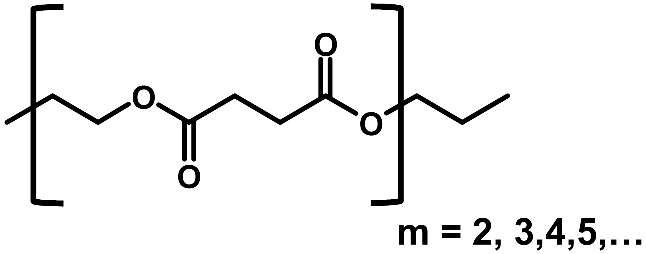
Rainer Buerstinghaus

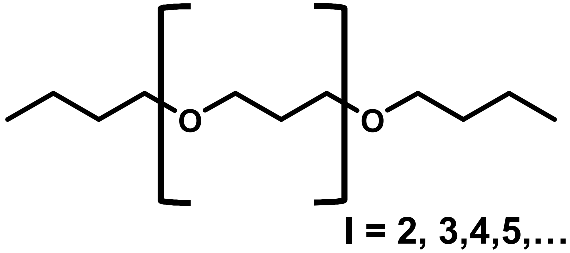
Electrodeposition Coatings for the Corrosion Protection of Car Bodies: CED Basic Resin (Simplified Representation).

Example



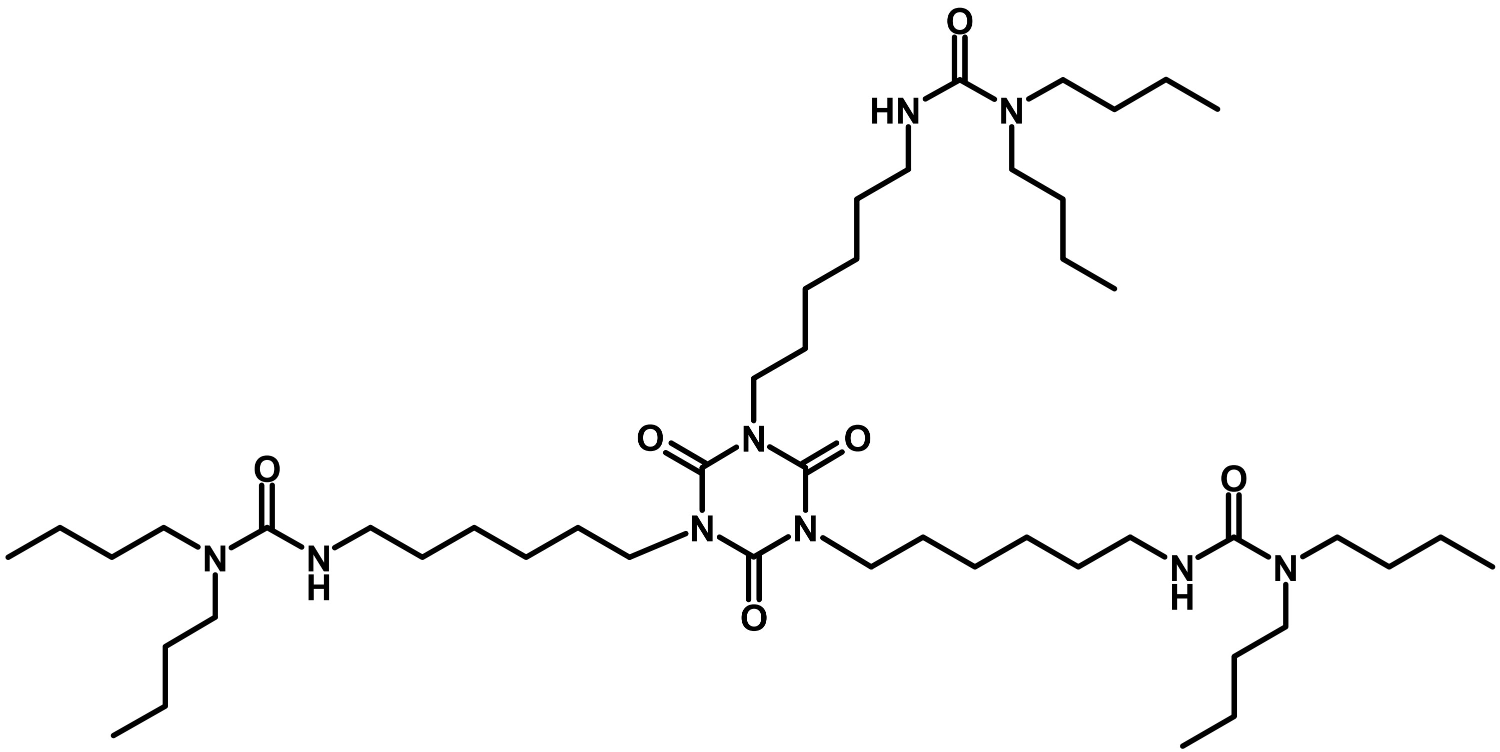
– R – = e. g. :





The protonated, amine-modified epoxy resin forms a stable, electrophoretically depositable secondary dispersion in water.

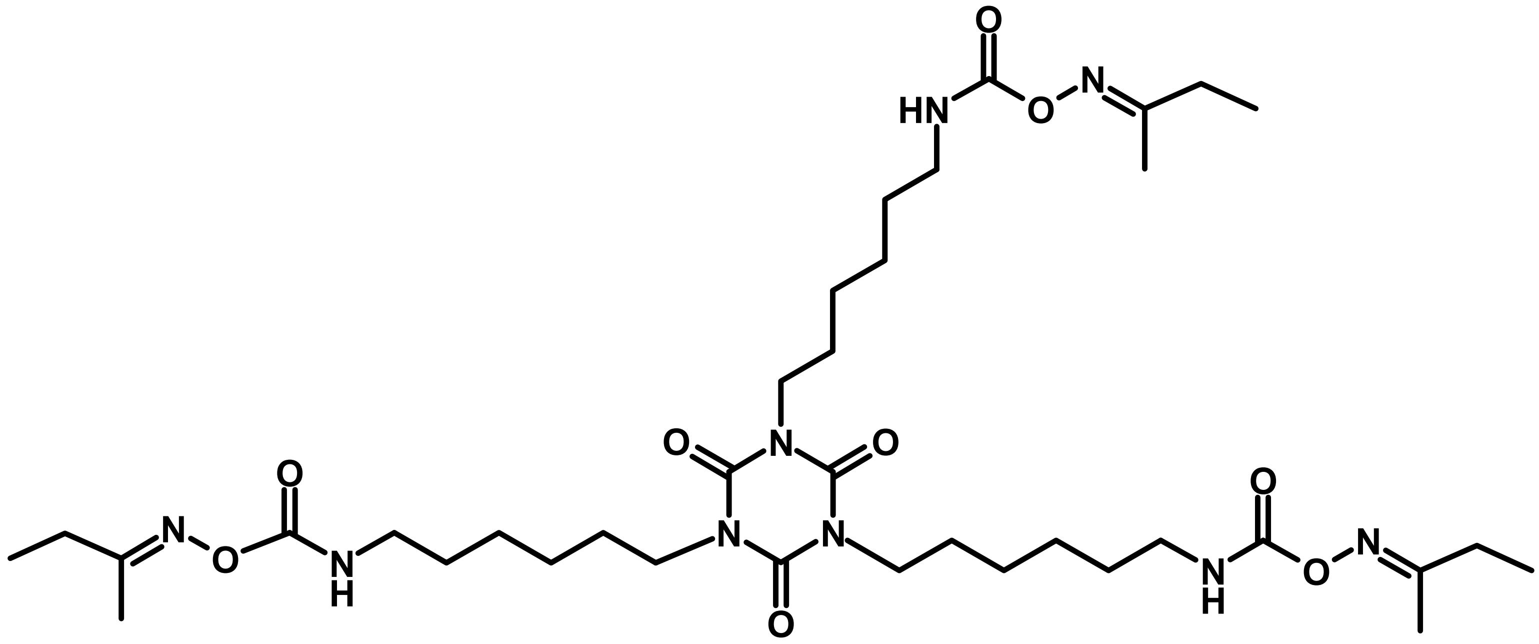
Electrodeposition Coatings for the Corrosion Protection of Car Bodies: Cross-Linking, Blocked Oligoisocyanate.



Temperature range for deblocking: 120ºC - 160ºC.

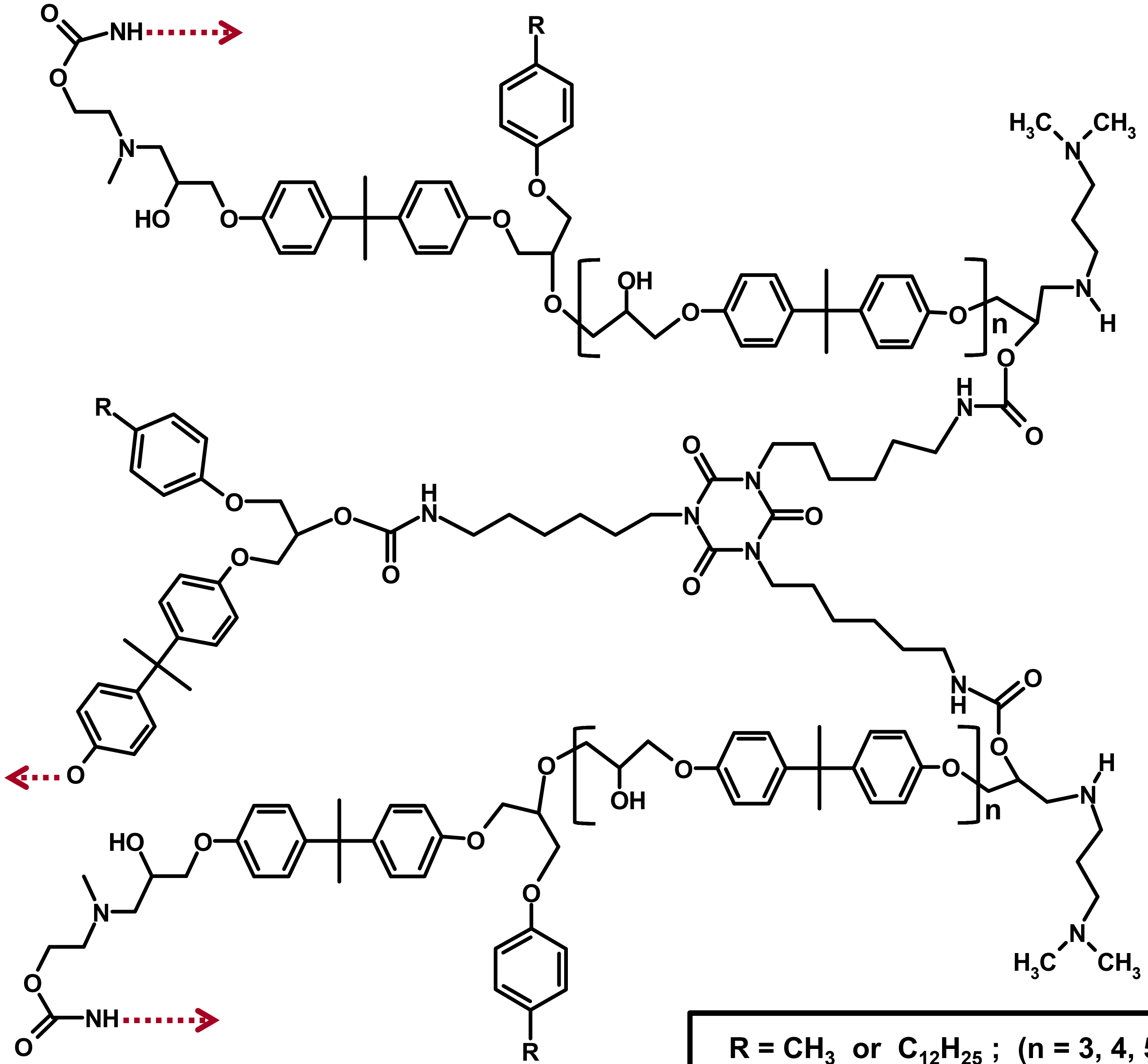
Rainer Buerstinghaus

Electrodeposition Coatings for the Corrosion Protection of Car Bodies: Cross-Linking, Blocked Oligoisocyanate.



Temperature for deblocking: round about 150ºC.

Electrodeposition Coatings for the Corrosion Protection of Car Bodies: CED Resin after Baking Process (Example).



R = CH_3 or $C_{12}H_{25}$; (n = 3, 4, 5…)

EC-Duromer

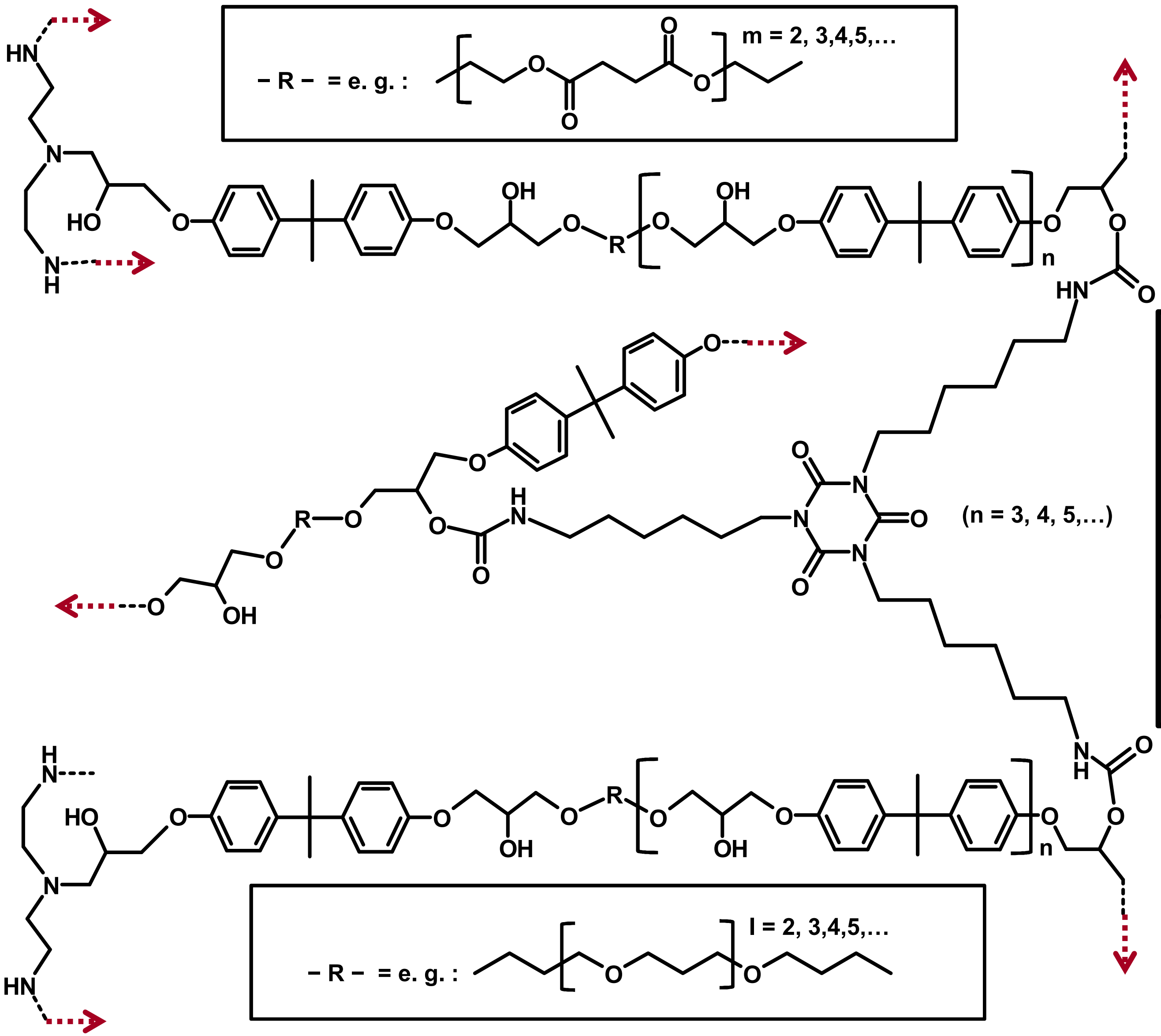
CED Basic Resin After Crosslinking by "Re-Urethanization". Detail from the Polymer Structure.

(Idealized Structure)

$T_{Cur.} \approx 185^oC$

Rainer Buerstinghaus

Electrodeposition Coatings for the Corrosion Protection of Car Bodies: CED Resin after Baking Process (Example).



EC-Duromer

CED Basic Resin After Crosslinking by "Re-Urethanization". Detail from the Polymer Structure.

(Idealized Structure)

$T_{Cur.} \approx 185^oC$

Rainer Buerstinghaus

Further literature (books, articles, patent specification) on the subject: "Electrodeposition Coatings for the Corrosion Protection of Car Bodies".

- H-J. Streitberger, K-F. Dössel, Automotive Paints and Coatings, Wiley-VCH, Weinheim, 2008.
- H. Reuter, W. Jouck, G. Ott, US-Pat. 575372A, BASF Coatings AG, 1996.
- L. Besra, M. Liu: A review on fundamentals and applications of electrophoretic deposition (EPD), Progress in Materials Science. ScienceDirect, 52(1), 2007. 1–61.
- M. Brahm, Polymerchemie kompakt, Hirzel, Stuttgart, Leipzig, 2016.
- H. Fobbe in: Kittel, Lehrbuch der Lacke und Beschichtungen, Band 9, Hirzel, Stuttgart, 2004.
- A. Goldschmidt, H-J. Streitberger, BASF Handbuch Lackiertechnik, Vincentz, Hannover, 2014.
- S. Koltzenburg, M. Maskos, O. Nuyken, Polymere, Springer Spektrum, Heidelberg 2014.
- B. Tieke, Makromolekulare Chemie, Wiley-VCH, Weinheim, 2014.
- M. Reichinger, W. Bremser, M. Dornbusch, Interface and volume transport on technical cataphoretic painting: A comparison of steel, hot-dip galvanised steel and aluminum alloy, Electrochimia Acta, 231, 135-152, 2017.
- T. Brock, M. Groteklaes, P. Mischke, Lehrbuch der Lacktechnologie, Vincentz, Hannover, 2017.
- P. F. W. Simon, A. Fahmi, Polymere - Chemie und Strukturen, Wiley-VCH, Weinheim, 2020.
- B. Müller, U. Poth, Lackformulierung und Lackrezeptur, Vincentz, Hannover, 2017.
- T. Brock, Elektrotauchlackierung, Chemie in unserer Zeit, 51, 300-307, 2017.

R&D Project Management
in the Chemical Industry

Supplementary Module 03 for Chemists (m/f/d)

Information Material *for the subject matter:*
Innovation, Classification of the Target Market.

"Solvent-Reduced NAD Lacquer for the Metal Forming-Resistant Inner Coating of Tinplate Cans."

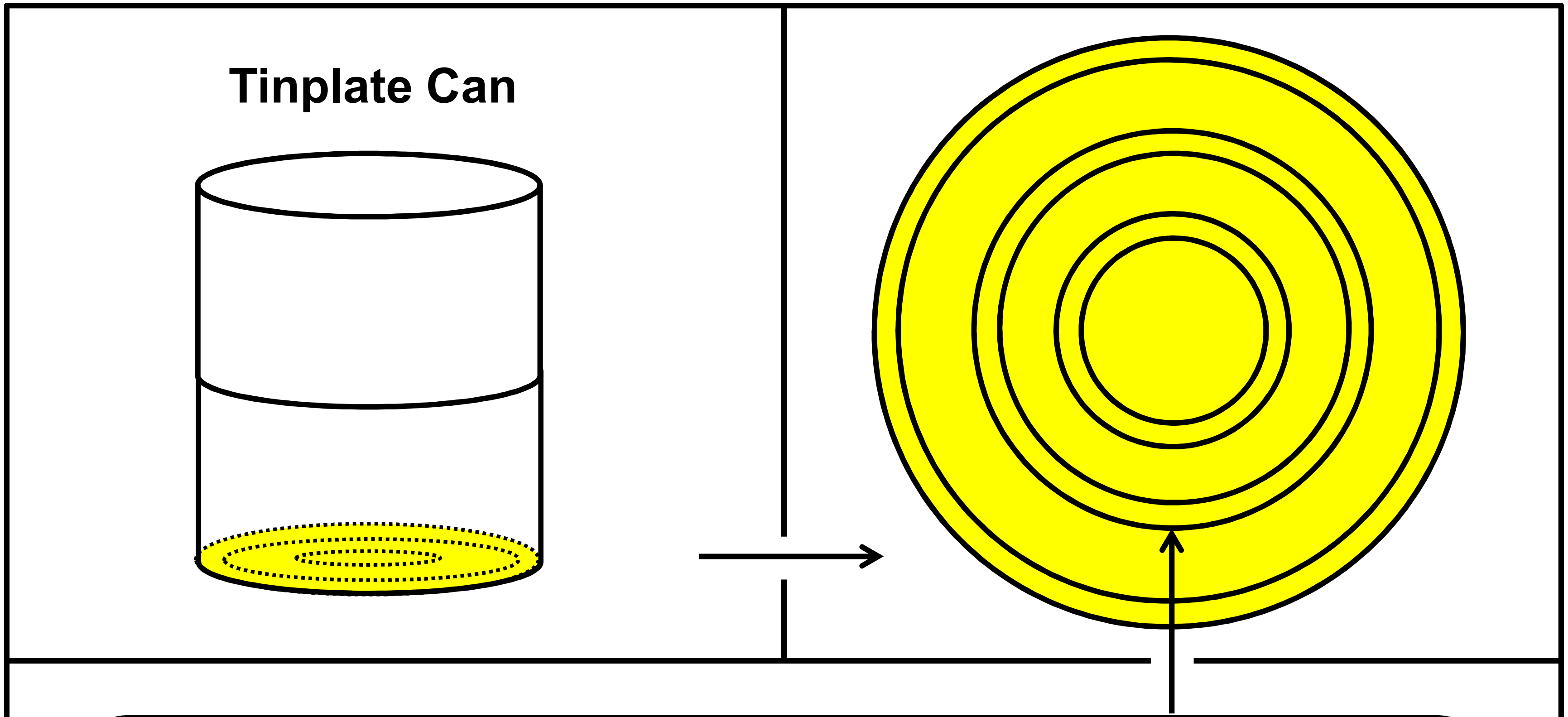
Rainer Buerstinghaus

R&D Project Management in the Chemical Industry

Subject Matter	***Innovation, Classification of the Target Market.***

Chemical-Technical Basics: "Solvent-Reduced NAD Lacquer for the Metal Forming-Resistant Inner Coating of Tinplate Cans."

"Gold-Coated" and Reshaped Base of the Tinplate Can.

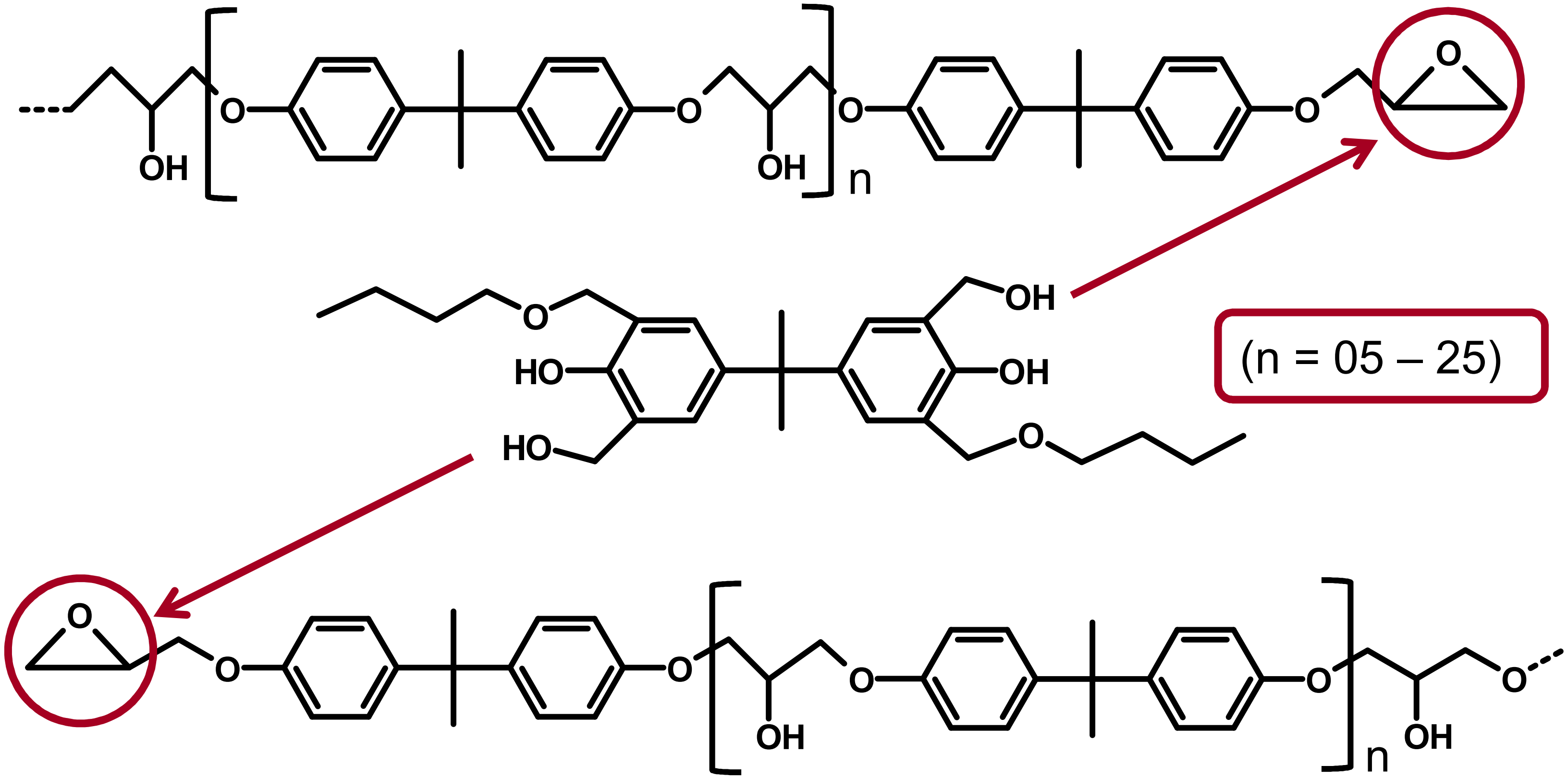


"Corrugation" to increase the rigidity / strength of bases for tinplate cans. The punching and forming are done ***after*** the painting of the flat tinplate.

Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

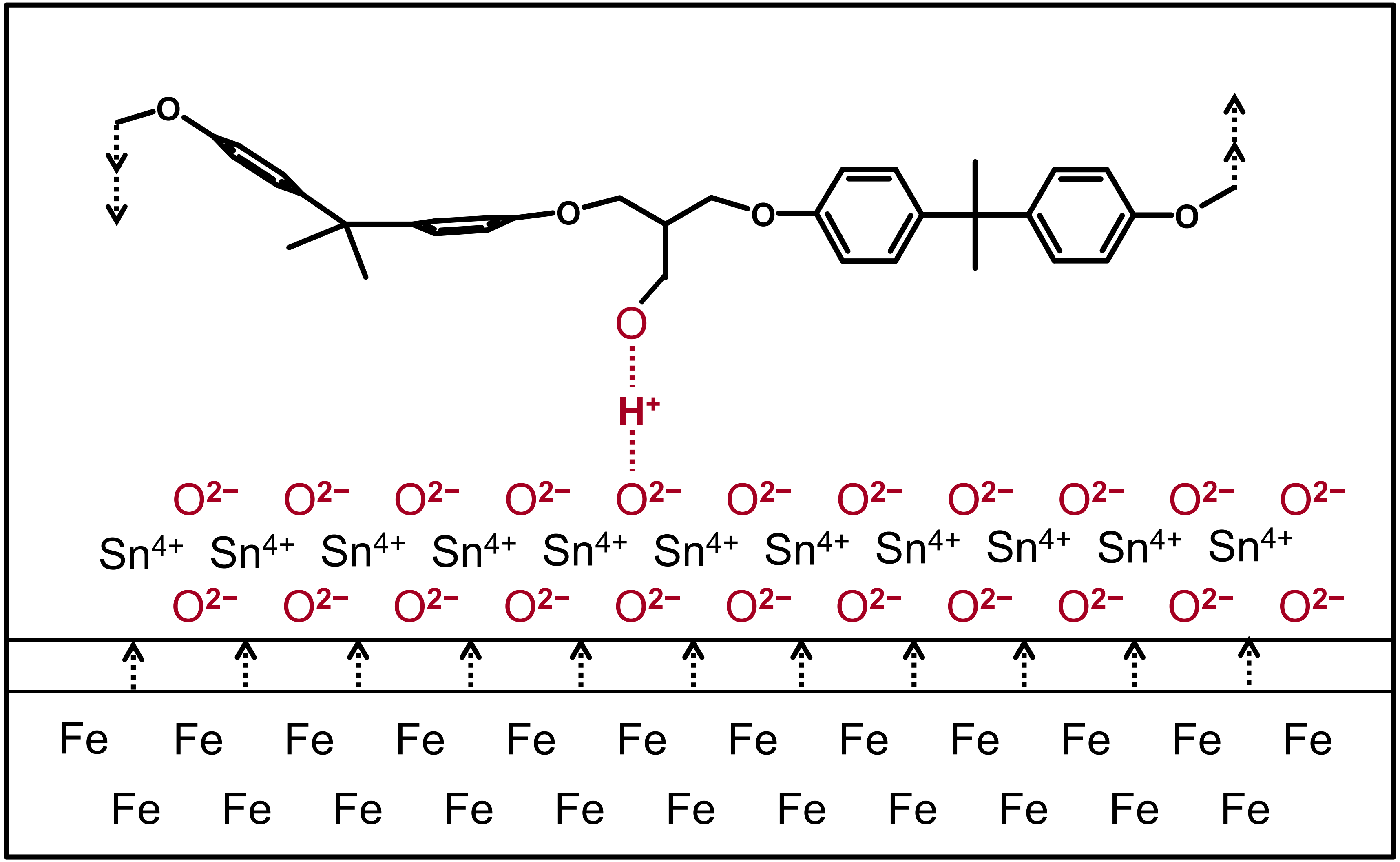
Resins for "Gold Lacquers", before Stoving:
Epoxy Resins and Phenol Formaldehyde Resin (Crosslinking).



Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

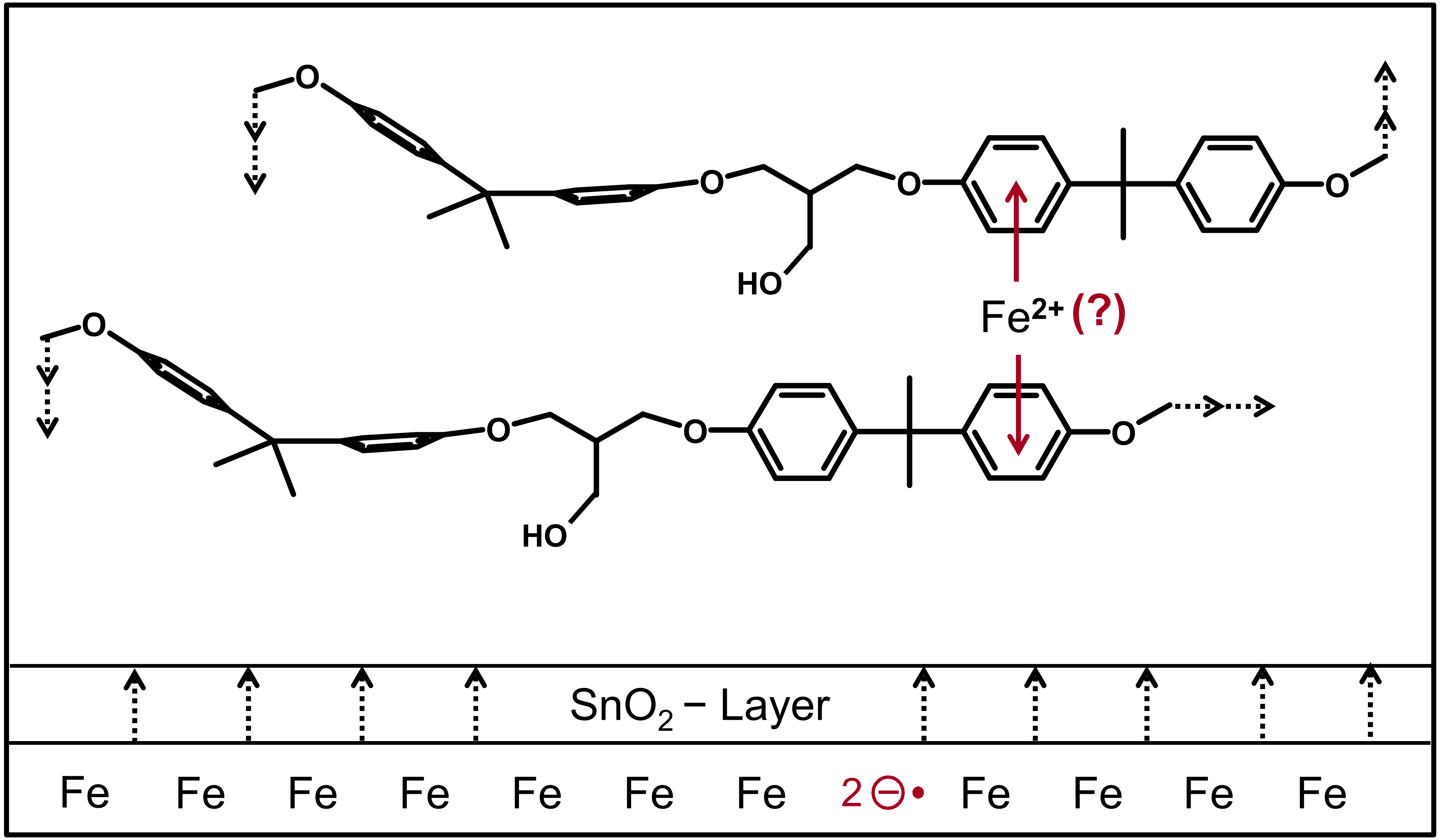
Tinplate, Coated with Epoxy-Phenolic Resin Duromer.
Corrosion Protection: Adhesion to the SnO_2-Layer via H^+-Bridges.



Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

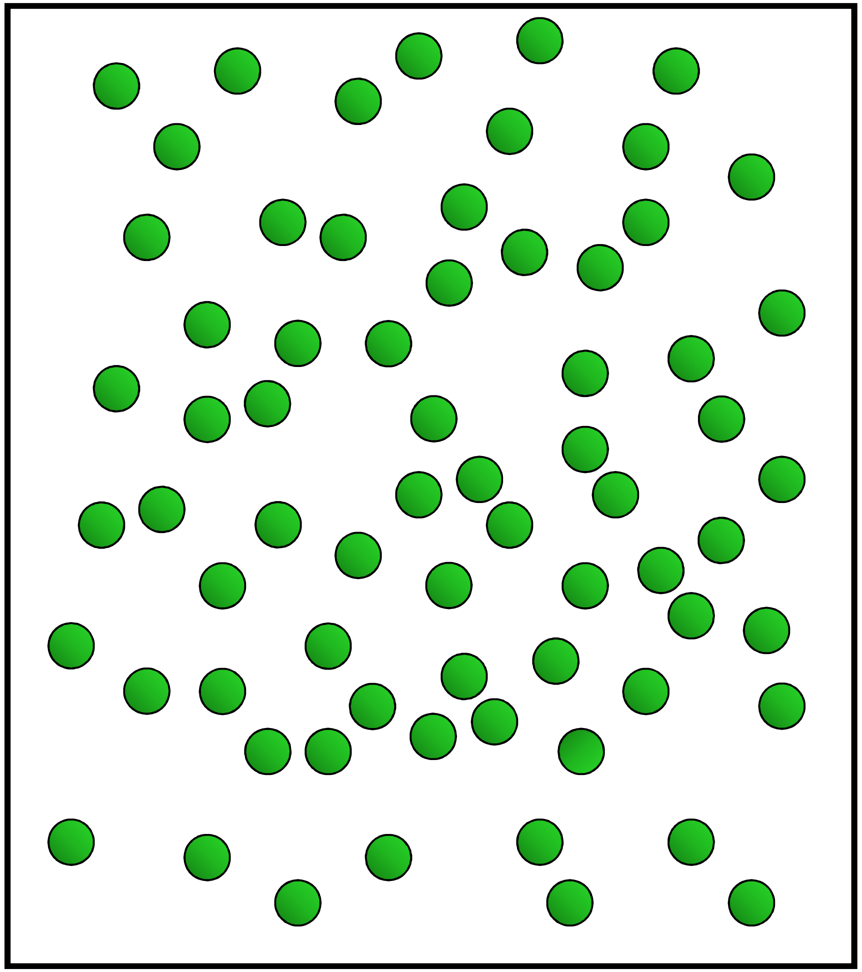
Corrosion Protection: Complexation of "Free" Fe^{2+}- Ions between Electron Rich, Aromatic Rings (?) (Idealized Representation).



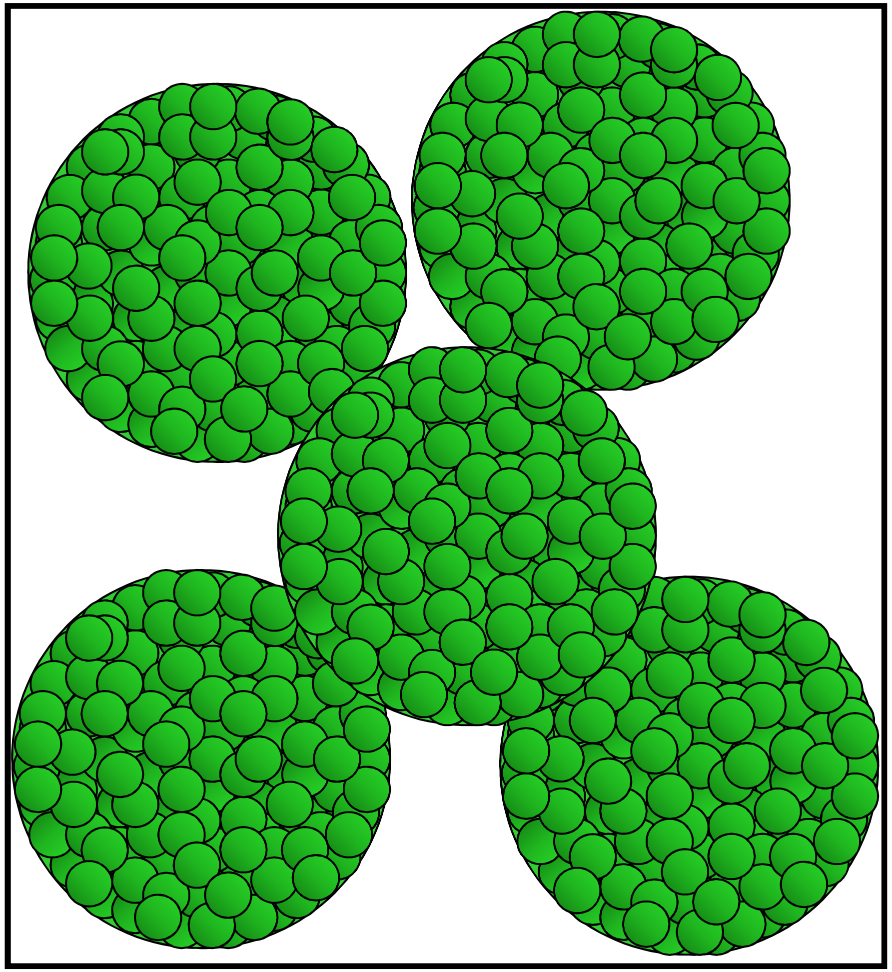
Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

PVC Dispersion as a “Lacquer Additive" to Raise the Solid Content.



Aqueous PVC Primary Dispersion

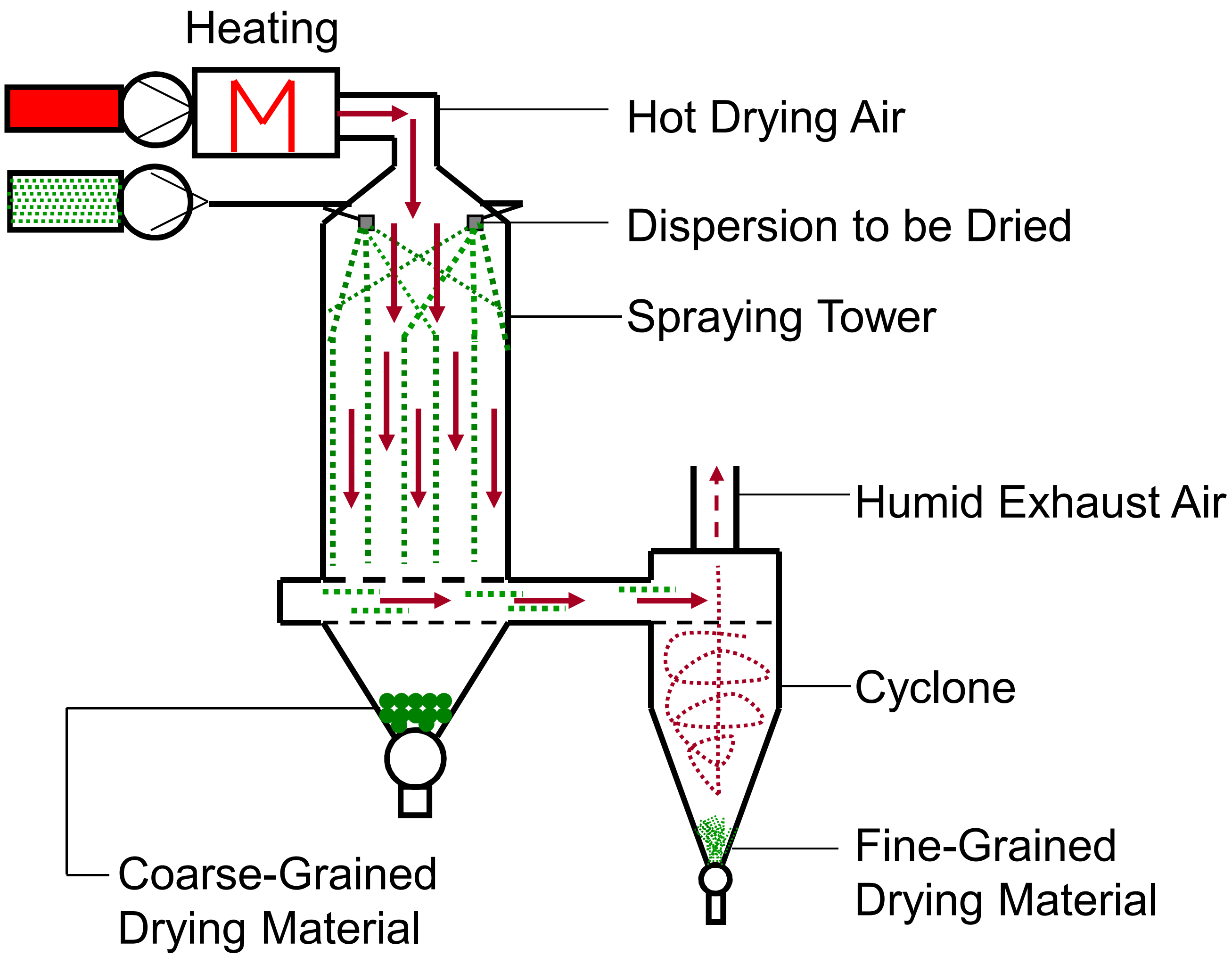


Spray-Dried Agglomerate

Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

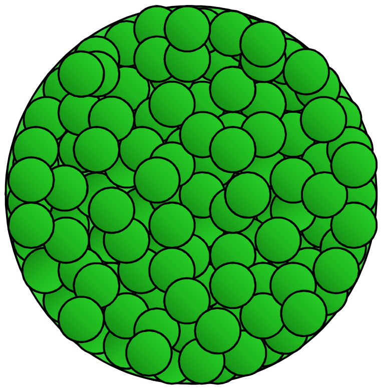
Spray-Dryer for Polymer Dispersions.



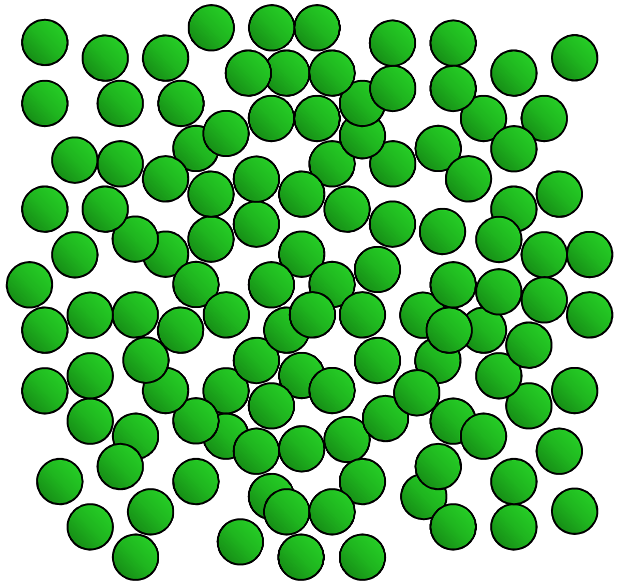
Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

Spray-Dried PVC Dispersion.



Spray-dried primary particle agglomerate

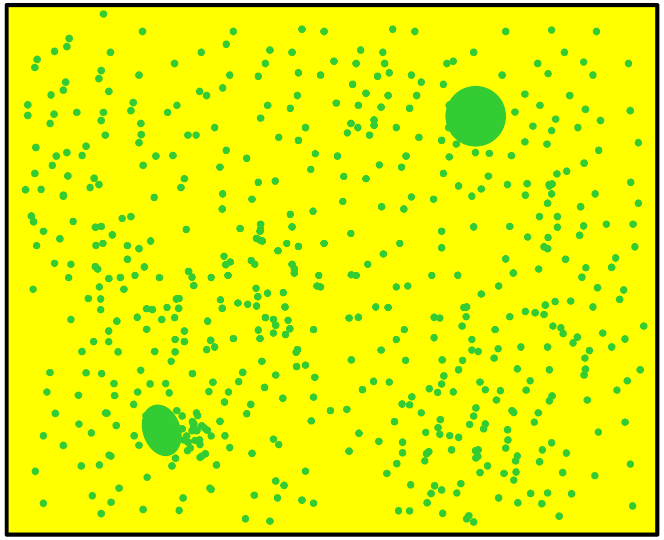


Primary particles in the wet preparation

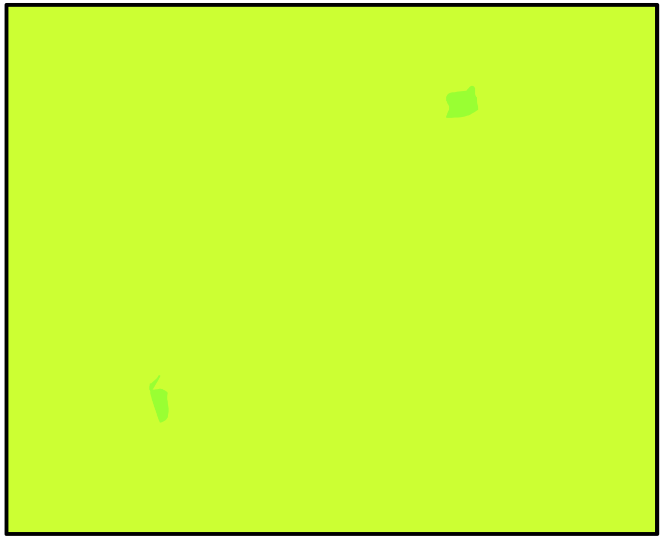
Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

Spray-Dried PVC Dispersion as an Additive for Gold Lacquers.



Wet preparation, transmitted light microscope, magnification: 600 times. Orthoplan, phase contrast.

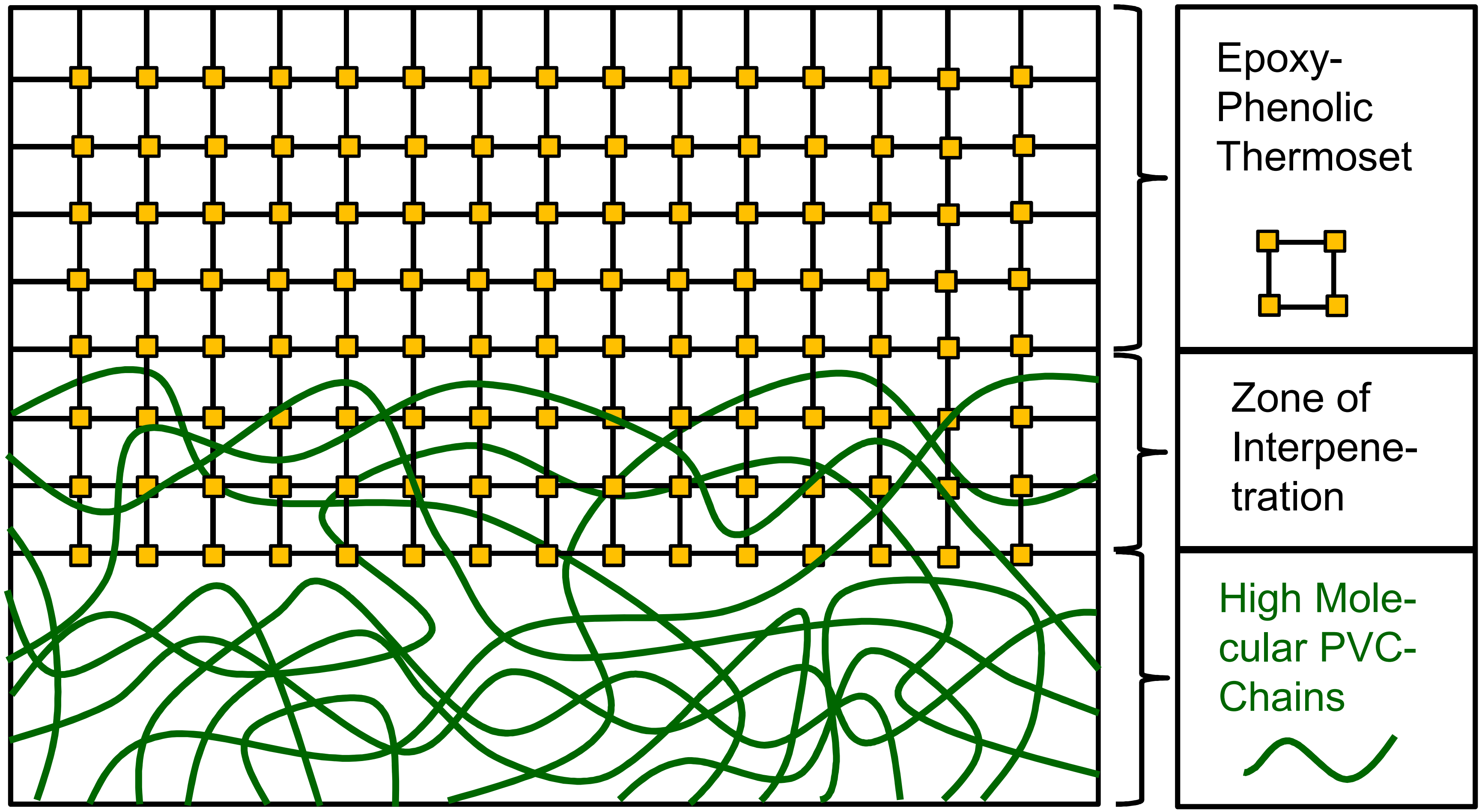


After 10 minutes at 210°C. magnification: 600 times. Orthoplan, phase contrast.

Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

"Interpenetrating Networks" after the Stoving of Tough-Elastic, Deep-Drawn Lacquer Films (Scheme).

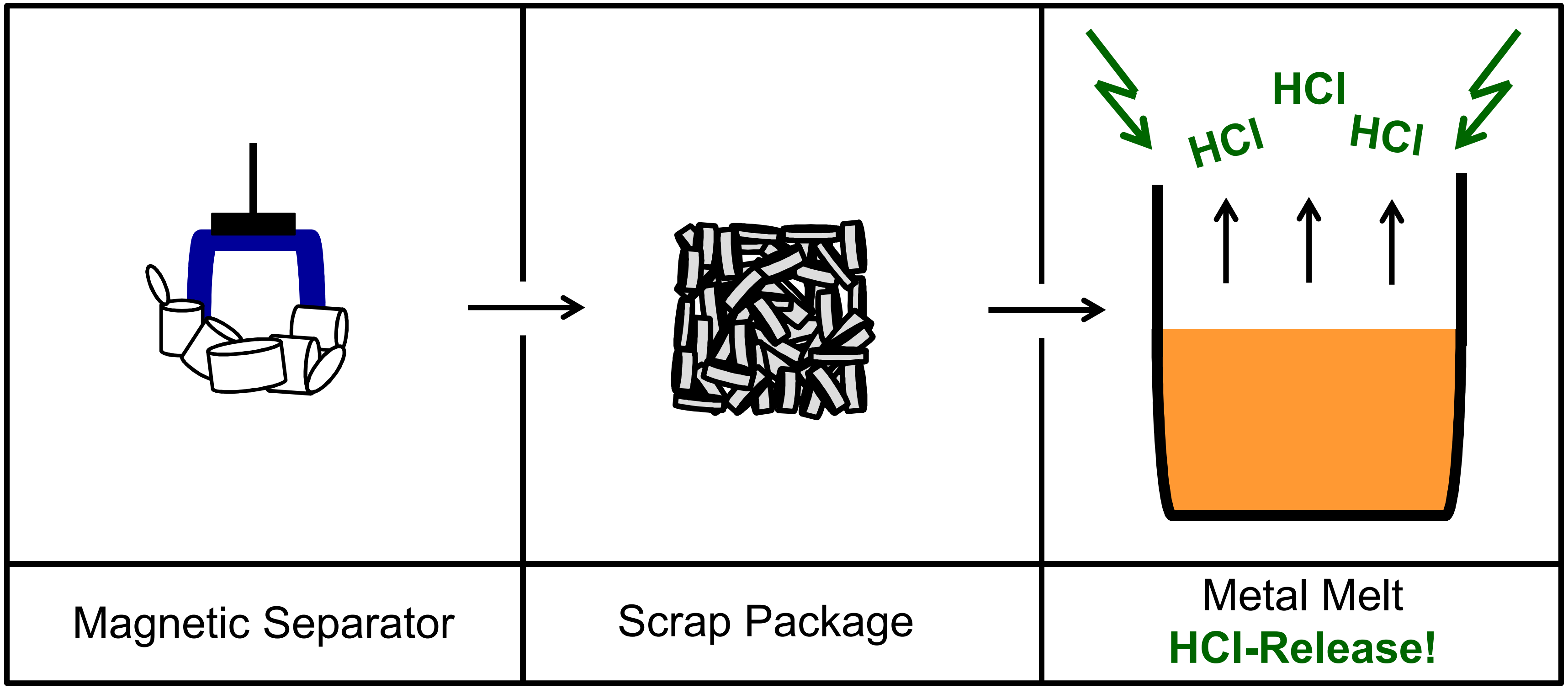


Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

Disadvantage when Recycling a PVC-Coated Can: HCl-Release!

1. Magnetic Separator	2. Scrap Package	3. Metal Melt
4. Slab-Cast	5. Cold Rolling	6. Galvanic Tin Plating
Tinplate Recycling Rate in Germany: 93%.		

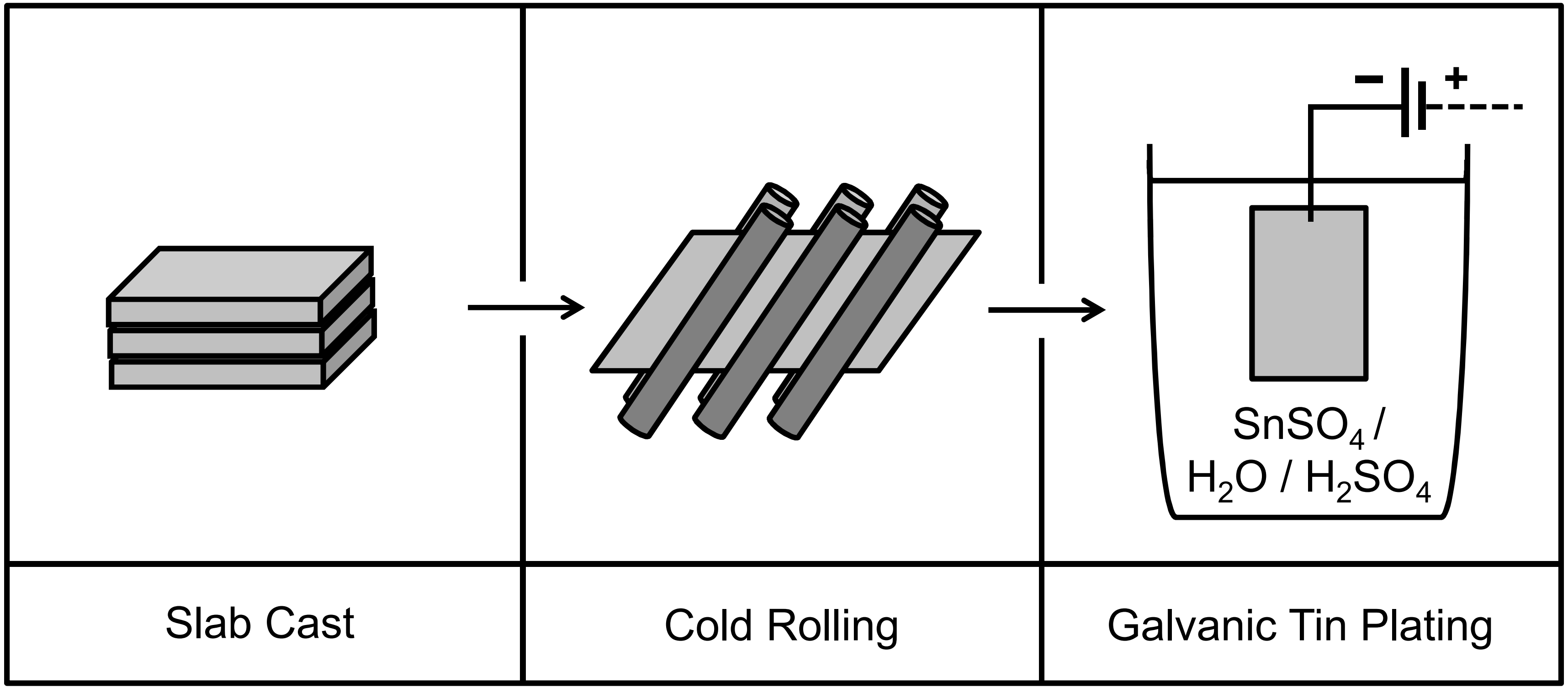


Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

Disadvantage when Recycling a PVC-Coated Can: HCl-Release!

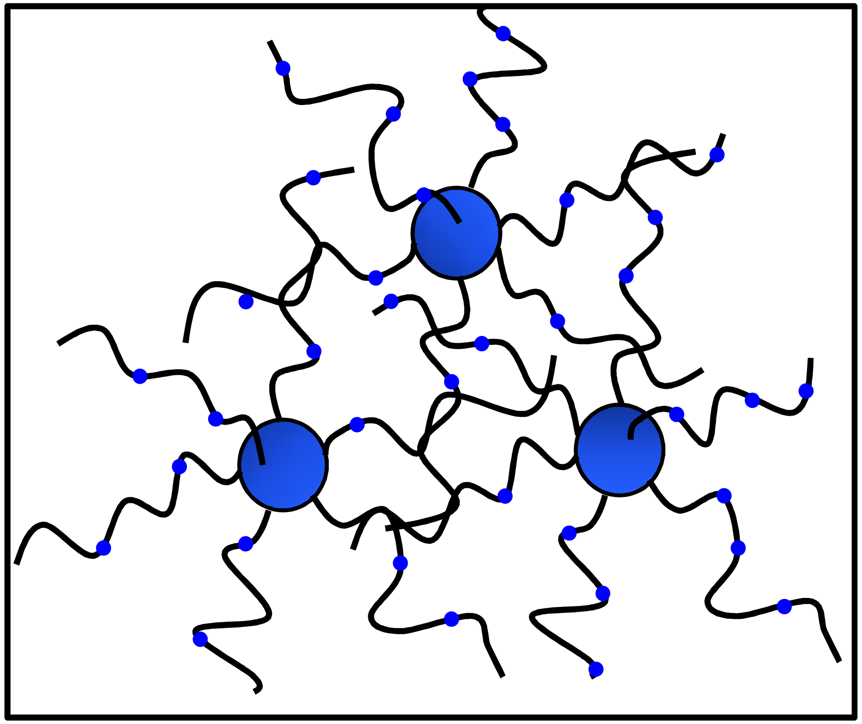
1. Magnetic Separator	2. Scrap Package	3. Metal Melt
4. Slab-Cast	5. Cold Rolling	6. Galvanic Tin Plating
Tinplate Recycling Rate in Germany: 93%.		

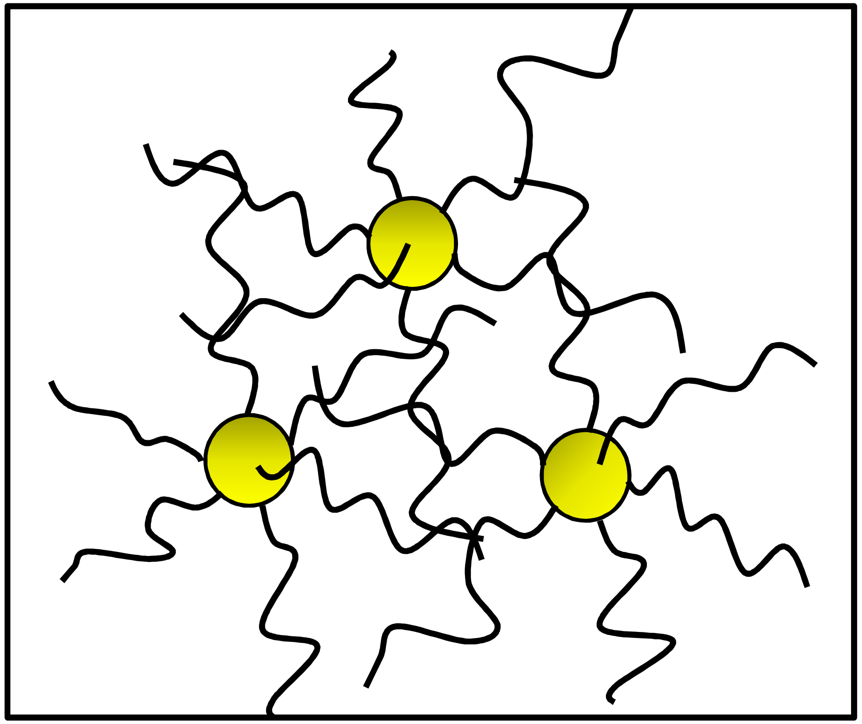


Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

Aqueous / Non Aqueous Dispersions, Structures.



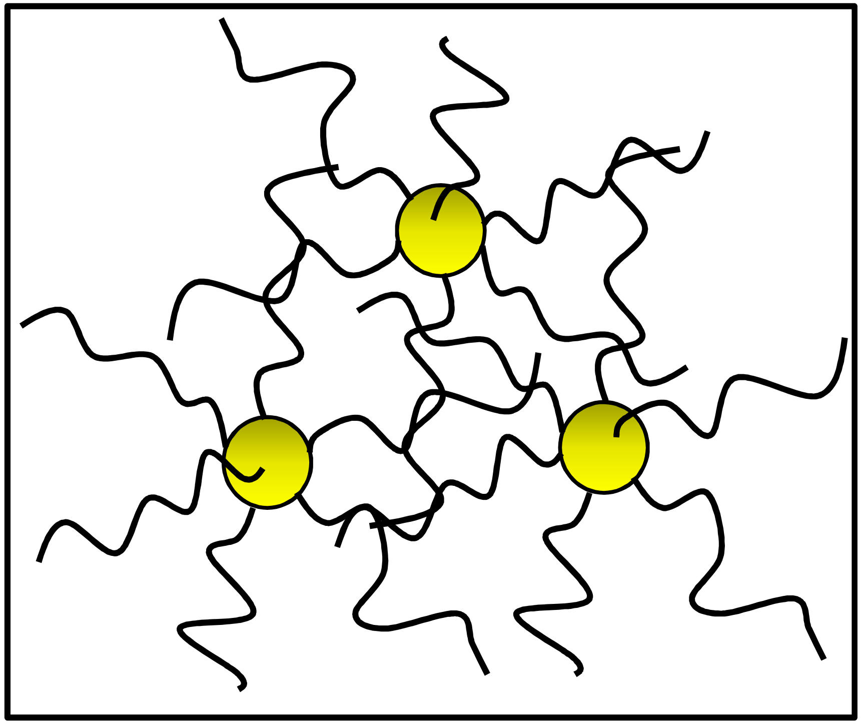


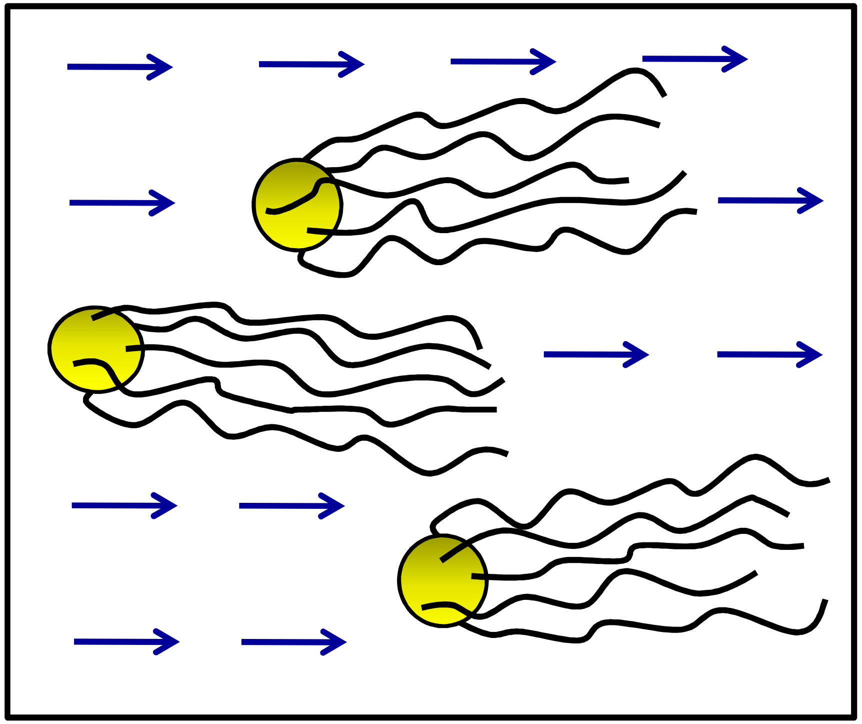
AD: Aqueous Dispersion	NAD: Non Aqueous Dispersion
• Hydrophilic structural elements. Polar + Steric Stabilization.	Non-polar groups. Purely Steric Stabilization.

Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

Thixotropy of a Non Aqueous Dispersion.



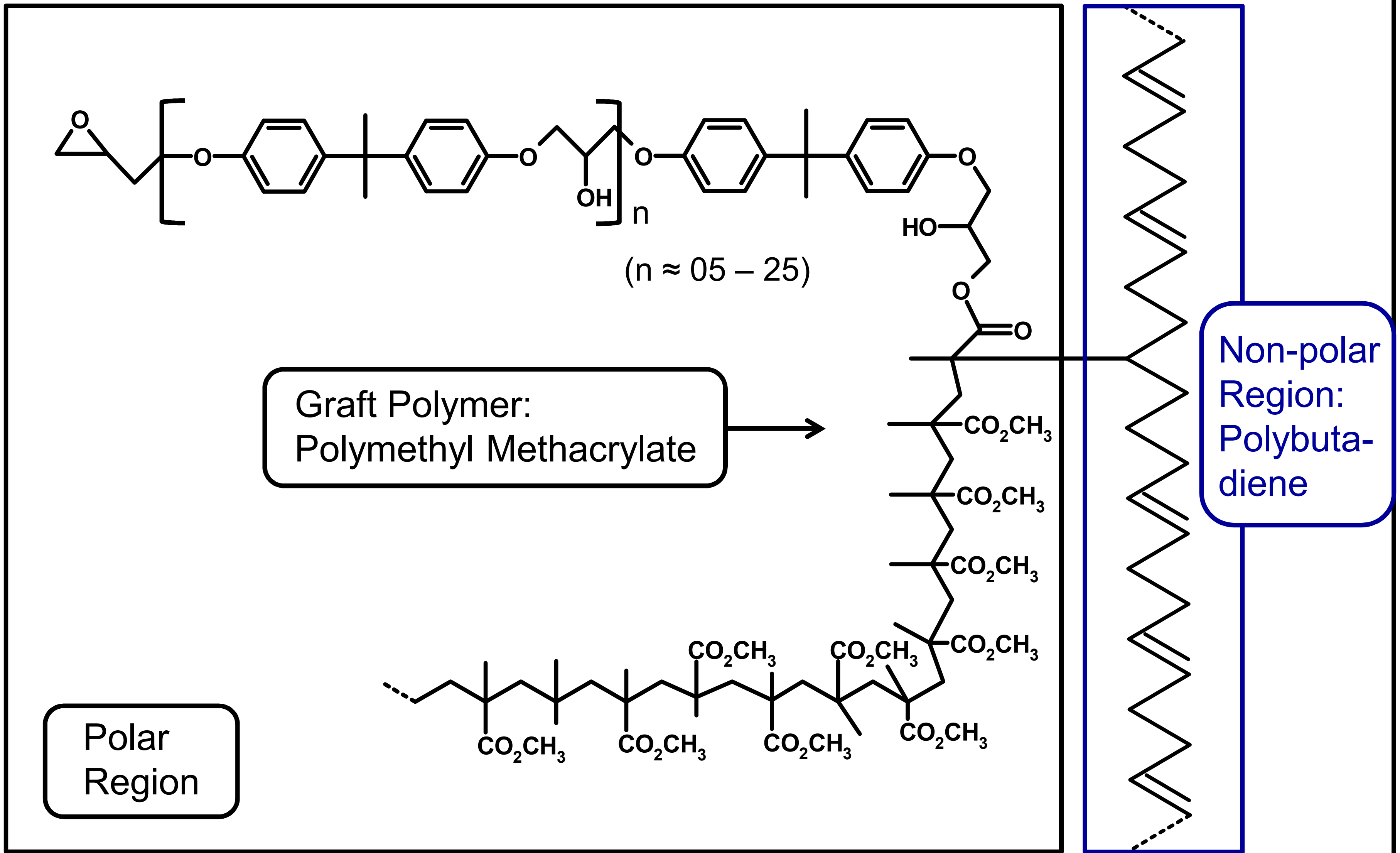


Gel-like and "stable".	Thin-liquid, easy to apply.
Low shear rate. High viscosity.	High shear rate. Low viscosity.

Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

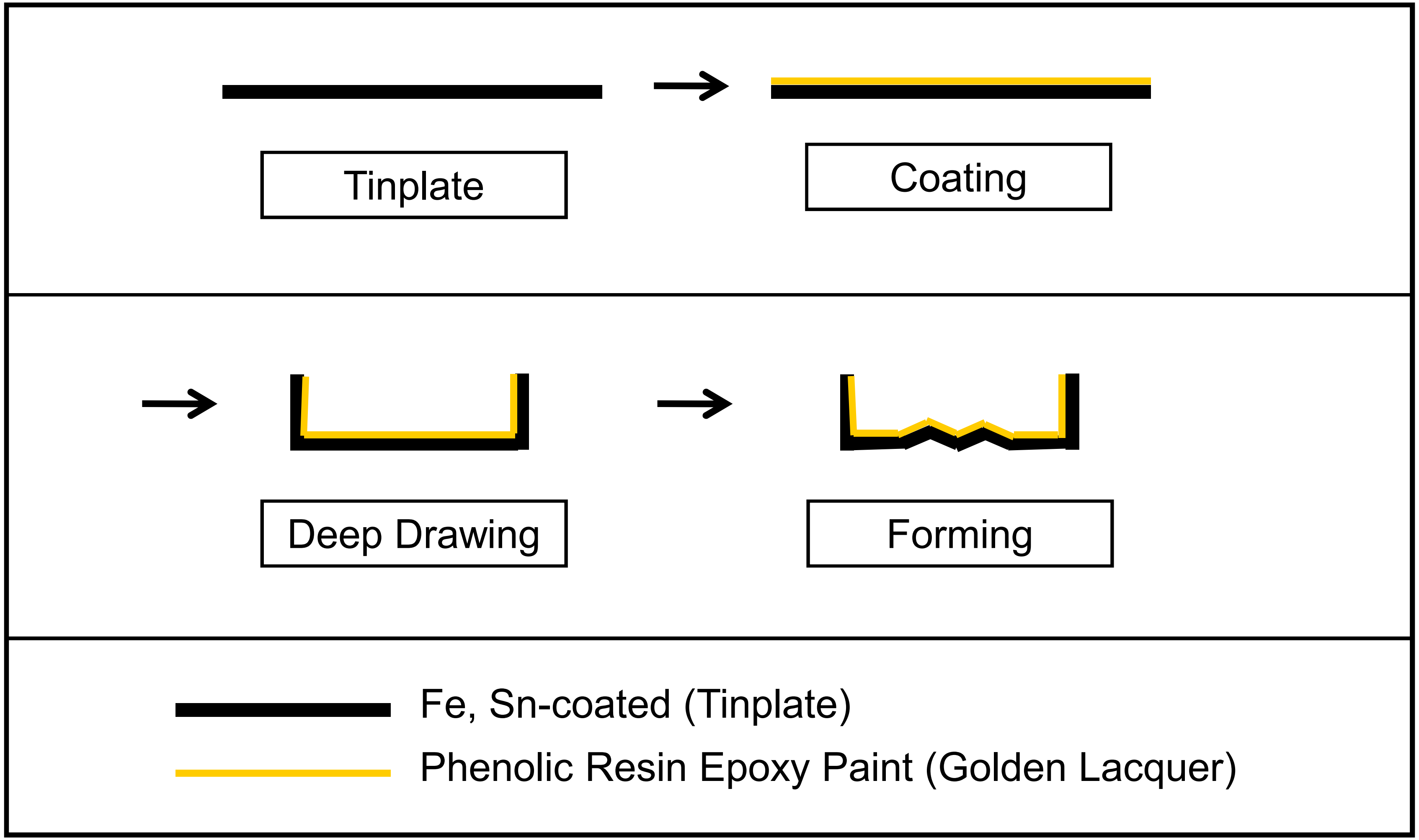
Epoxy Resin - NAD, PVC-Free, PMMA Graft Adduct (Idealized).



Rainer Buerstinghaus

"Solvent-Reduced NAD Lacquer…Coating of Tinplate Cans."

Deep Drawing and Forming of Coated Tinplates for Cans.



Rainer Buerstinghaus

Product Innovations, Market positions

Example

"NAD-Gold Lacquer" for the Coating of Tinplate Cans

Demand / *Competition*	strong	weak
strong	**Mass Markets** NAD-Gold Lacquer →	**Shrinking Markets** (*)
weak	**Future Markets**	**Niche Markets**

(*) Slight Trend towards Shrinking Market (Legislation).

Rainer Buerstinghaus

Further literature (specialist books, patent specifications) on the subject: "Solvent-Reduced NAD Lacquer for the Inner Coating of Tinplate Cans".

- K.-H.Scherping, J.Hölscher, U. Reichelt, U. Reiter, WO/1988/001287, BASF Lacke + Farben AG.
- A. Schmitz, L. Vogdanis, EP19970108416, BASF Coatings AG, 1997.
- M. Brahm, Polymerchemie kompakt, Hirzel, Stuttgart, Leipzig, 2016.
- Kittel, Lehrbuch der Lacke und Beschichtungen, Band 2: W. Krauß: Bindemittel für lösemittelhaltige und lösemittelfreie Systeme, Hirzel, Stuttgart, Leipzig, 1998.
- A. Goldschmidt, H-J. Streitberger, BASF Handbuch Lackiertechnik, Vincentz, Hannover, 2014.
- S. Koltzenburg, M. Maskos, O. Nuyken, Polymere, Springer Spektrum, Heidelberg, 2014.
- B. Tieke, Makromolekulare Chemie, Wiley-VCH, Weinheim, 2014.
- M. D. Lechner, K. Gehrke, E. H. Nordmeier, Makromolekulare Chemie, Springer-Spektrum, Heidelberg, Berlin 2014.
- C. Wrana, Polymerphysik, Springer-Spektrum, Heidelberg, Berlin, 2014.
- B. Müller, U. Poth, Lackformulierung und Lackrezeptur, Vincentz, Hannover, 2017.
- T. Brock, M. Groteklaes, P. Mischke, Lehrbuch der Lacktechnologie, Vincentz, Hannover, 2017.
- P. F. W. Simon, A. Fahmi, Polymere - Chemie und Strukturen, Wiley-VCH, Weinheim, 2020.
- N. Kopytziok, Handbuch für die Umwelt- und Abfallberatung, Bundesverband für Umweltberatung, Würzburg, 2005.
- Praxishandbuch Korrosionsschutz: Vorsorgen – Behandeln – Konservieren. HFFI Verlag, Königswinter, 2014.

R&D Project Management
in the Chemical Industry

Supplementary Module 03 for (Physico)Chemists (m/f/d)

Information Material *for the subject matter:*
Physico-chemical basics for solving a ***Case Study Task****.*

N-Heterocyclic Compounds for Organic Light-Emitting Diodes, "OLEDs".

Rainer Buerstinghaus

R&D Project Management in the Chemical Industry

Subject Matter	***Physico-Chemical Basics (Task for a Case Study).***

N-Heterocyclic Compounds for Organic Light-Emitting Diodes, "OLEDs".

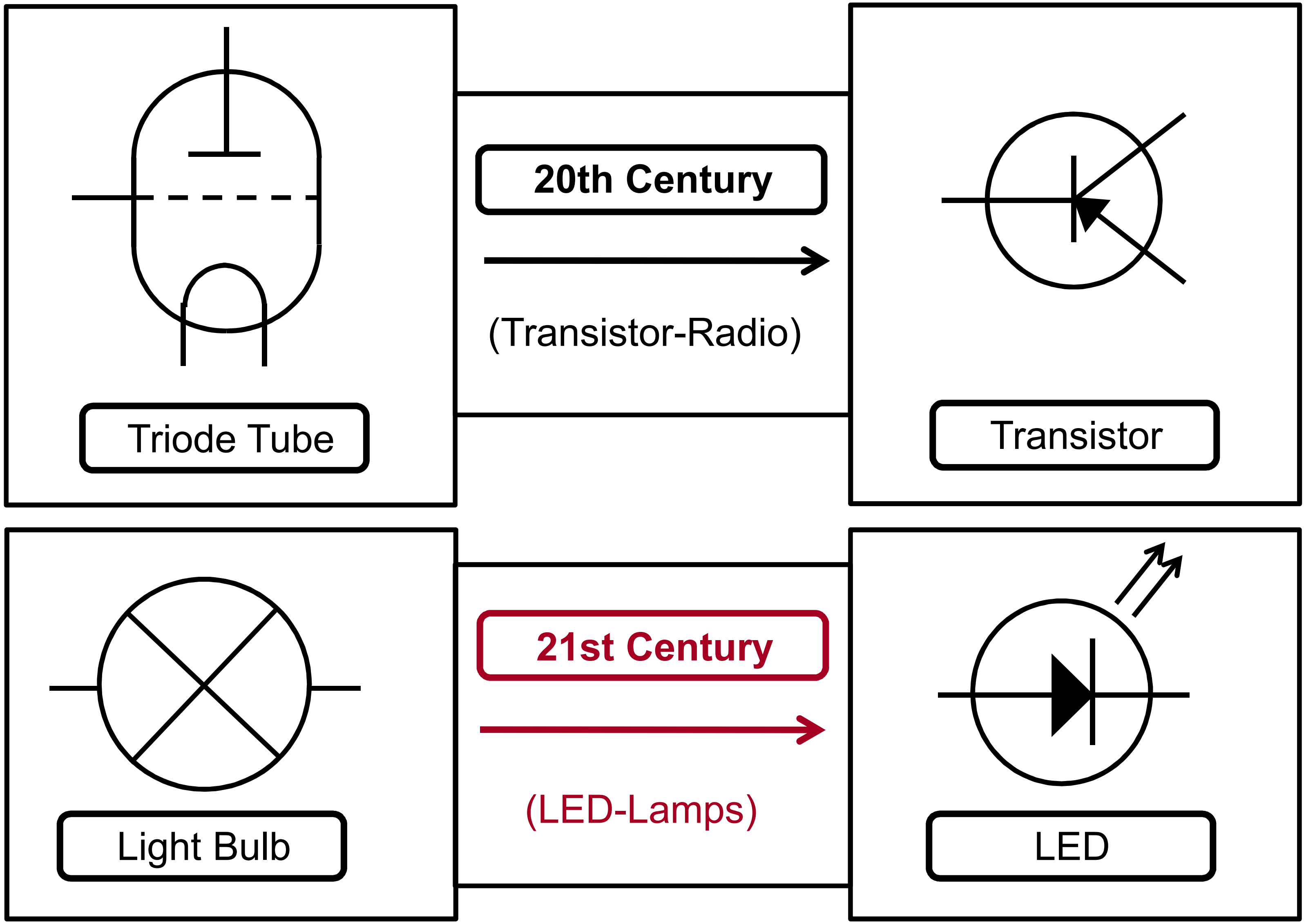
Rainer Buerstinghaus

History of Publicly Used Illuminants.

Year	Illuminants	Material	Innovators
1805	Gas Lamp	Natural Gas	English Entrepreneurs
1854	Bulb	Charred Strip of Bamboo	H. Goebel Hanover
1879	Bulb	Carbon Filament	T. A. Edison Menlo Park
1889	Bulb	Metal Filament Os / W	Auer von Welsbach Wien, Berlin
1926	Fluorescent Tube	Hg / ZnS	E. Germer, Berlin G.E. buys the Patent
1961	Inorganic Light Emitting Diode	GaN	N. Holonyak General Electric
1986	Organic Light Emitting Diode	Aluminum-Oxinate	Ching W. Tang Eastman-Kodak

N-Heterocyclic Compounds for OLEDs

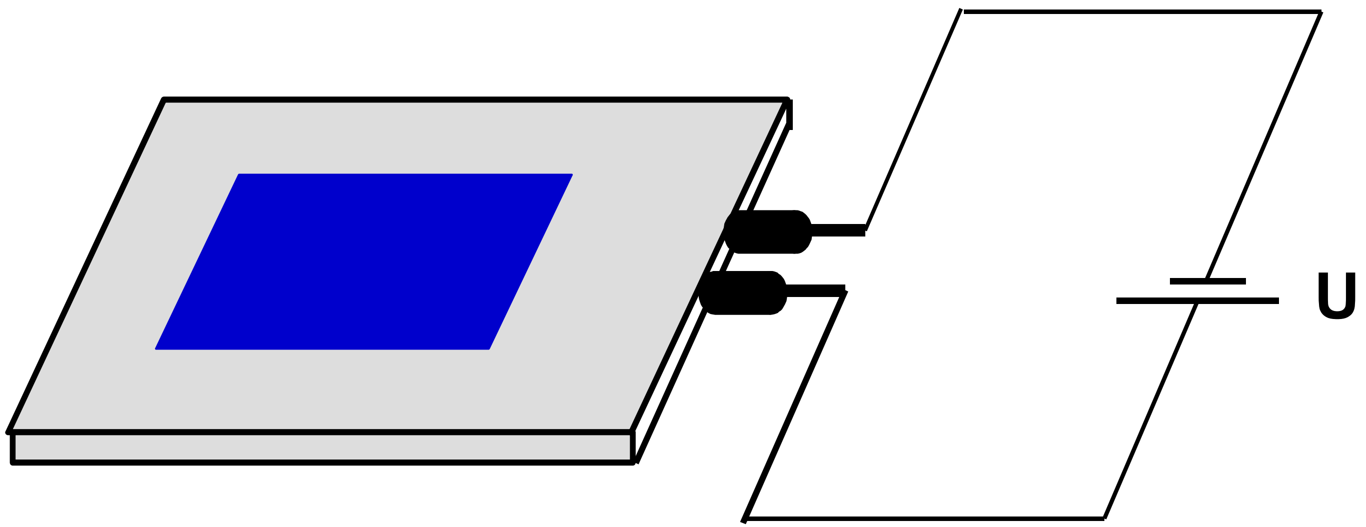
The "Lighting Revolution" in the 21st Century.



Rainer Buerstinghaus

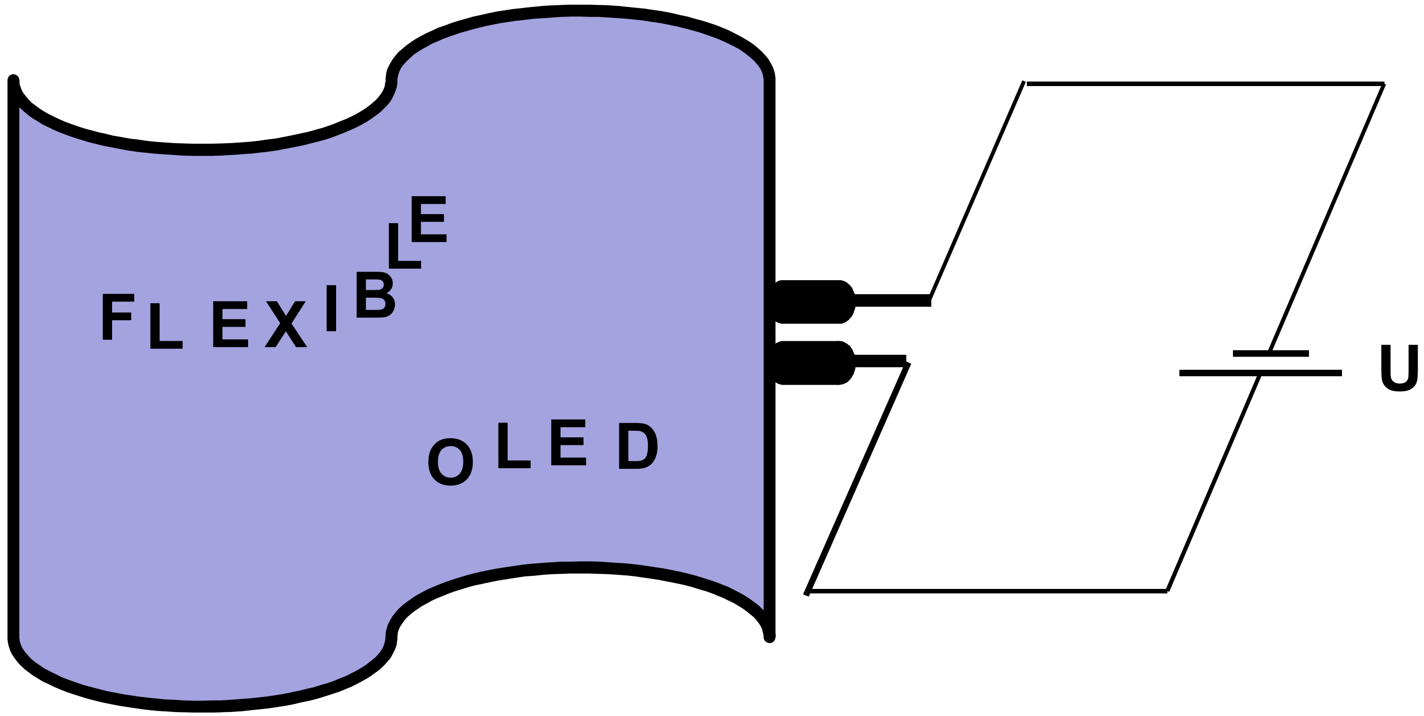
N-Heterocyclic Compounds for OLEDs

Organic Light Emitting Diode (Blue Emitter), Sketch.



Rainer Buerstinghaus

Flexible OLED on a Carrier Polymer, Sketch.



N-Heterocyclic Compounds for OLEDs

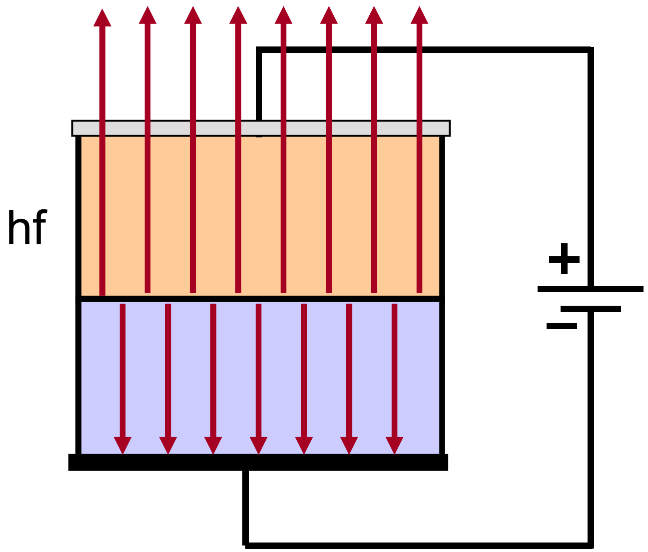
Advantages of Organic Light Emitting Diodes:

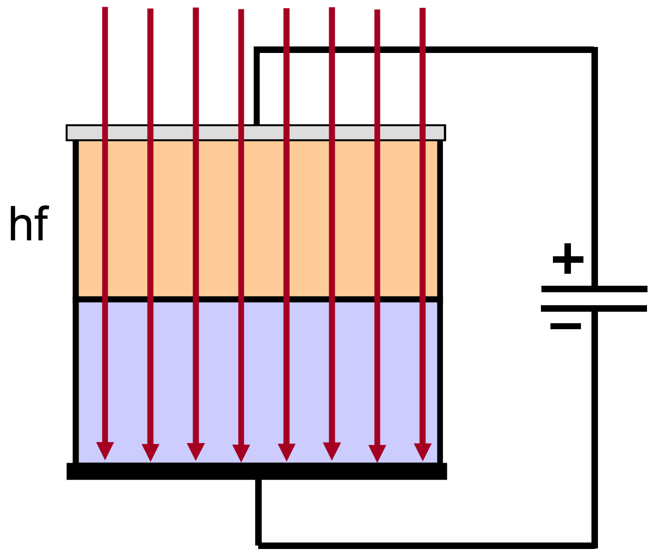
- Flat, diffuse, glare-free light source with a wide range of uses.
- Can be applied over a large area, large screen dimensions possible.
- High contrast (100:1), wide viewing angle.
- Low power consumption with high luminous efficacy (30 lm/W).
- Fast switching response, suitability for multimedia applications.
- Light, thin, flexible (without carrier material).

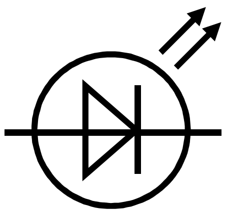
Current Problems with Organic Light Emitting Diodes:

- The lifespan must be improved (> 100,000 h).
- Sensitivity to water and oxygen.
- The total thickness with carrier material is too high: 1.8 mm.

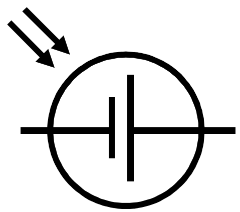
Inverse Physical Functional Principle of Two Optoelectronic Components.







LED:
Light emission at current flow.



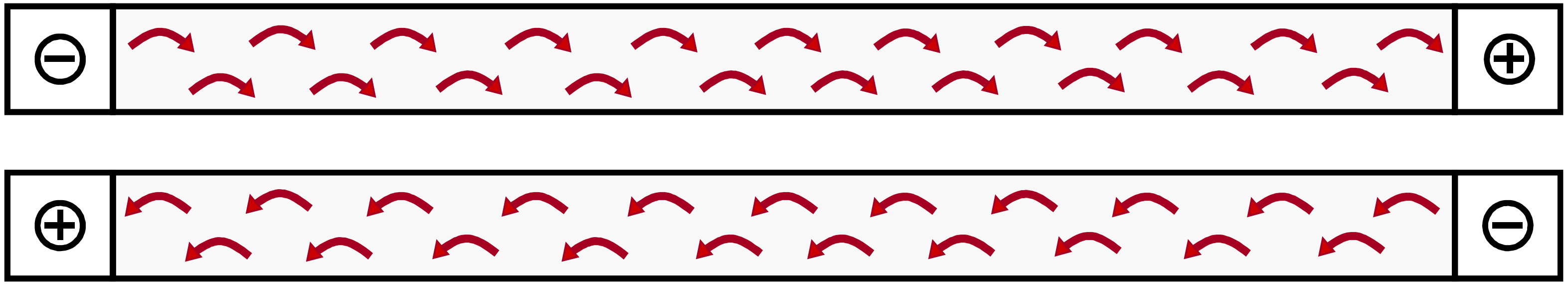
Photocell:
Current flow at incident light.

Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

Electrical Conductors, Semiconductors and Insulators.

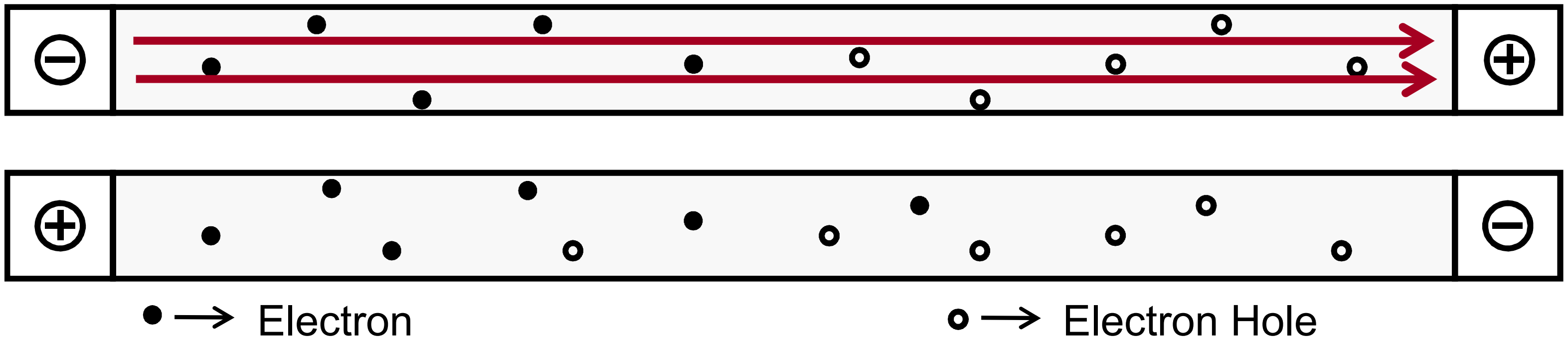
Electrical conductor: Almost "homogeneous" electron migration.



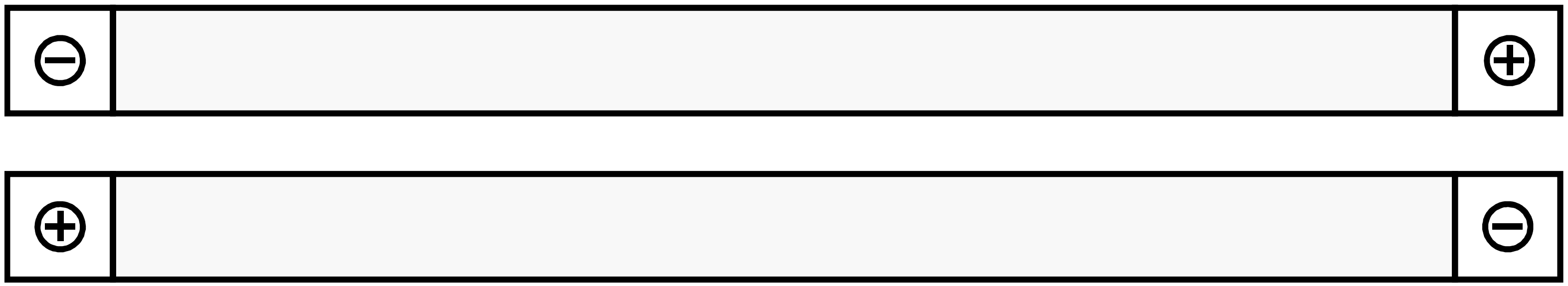
Semiconductors, undoped: "saltatory" electron migration.

Rainer Buerstinghaus

Electrical Conductors, Semiconductors and Insulators.



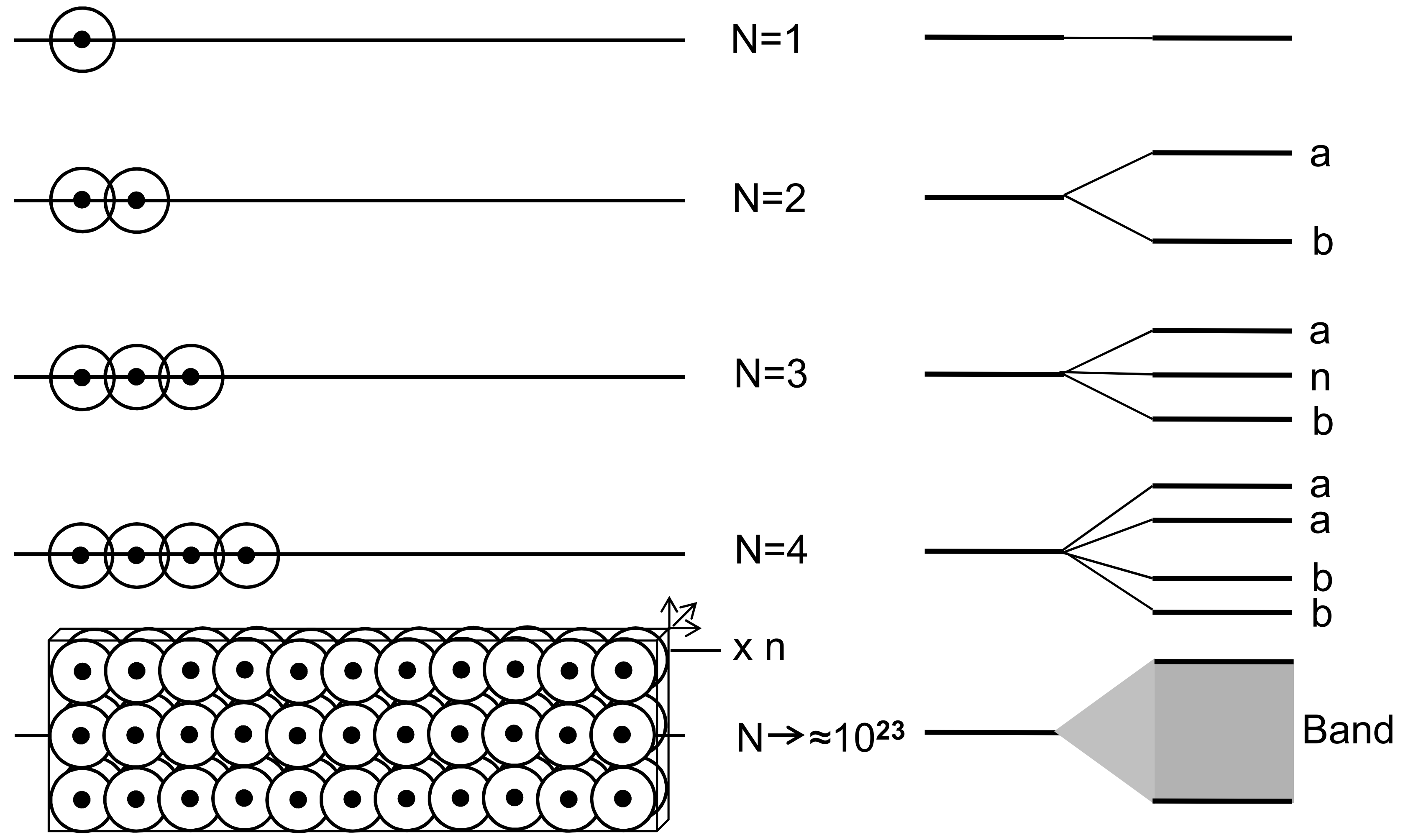
Semiconductors, border zone with n, p-doping: *Rectifier effect.*



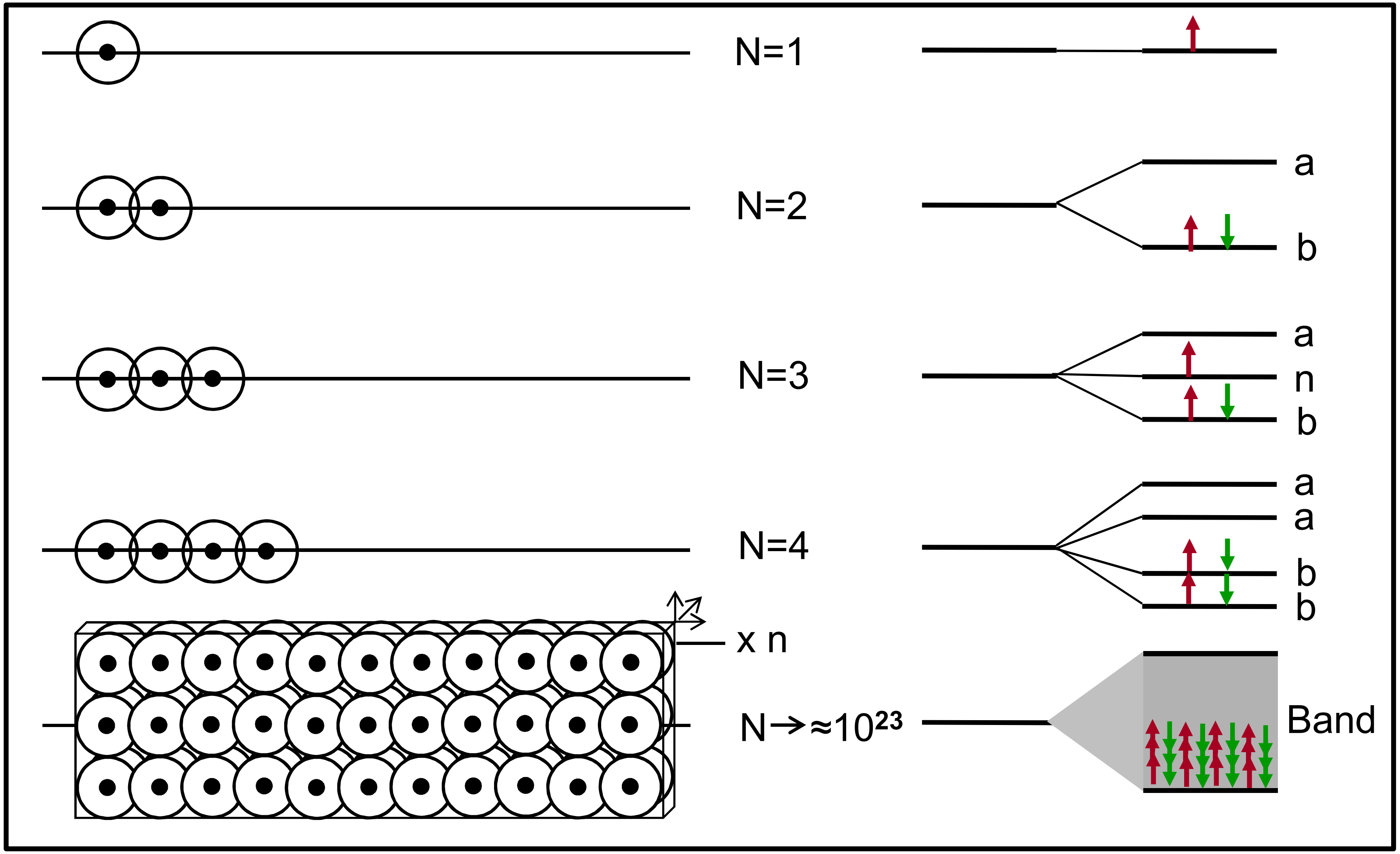
Electrical insulator: *No measurable electron migration.*

Rainer Buerstinghaus

Electrical Properties of Solids: Band Model for Periodic Multi-Atom Arrangements (Idealized).



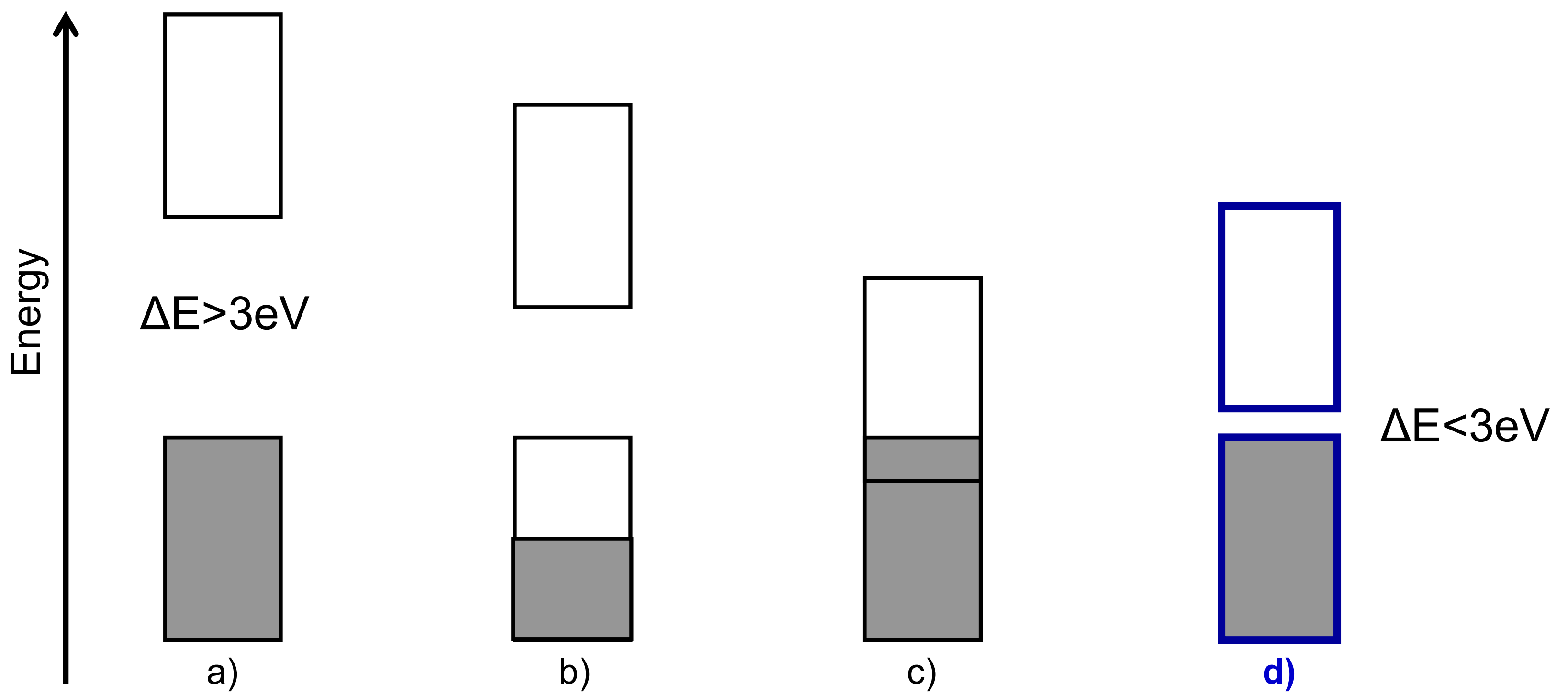
Electrical Properties of Solids: Band Model for Periodic Multi-Atom Arrangements (idealized).



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

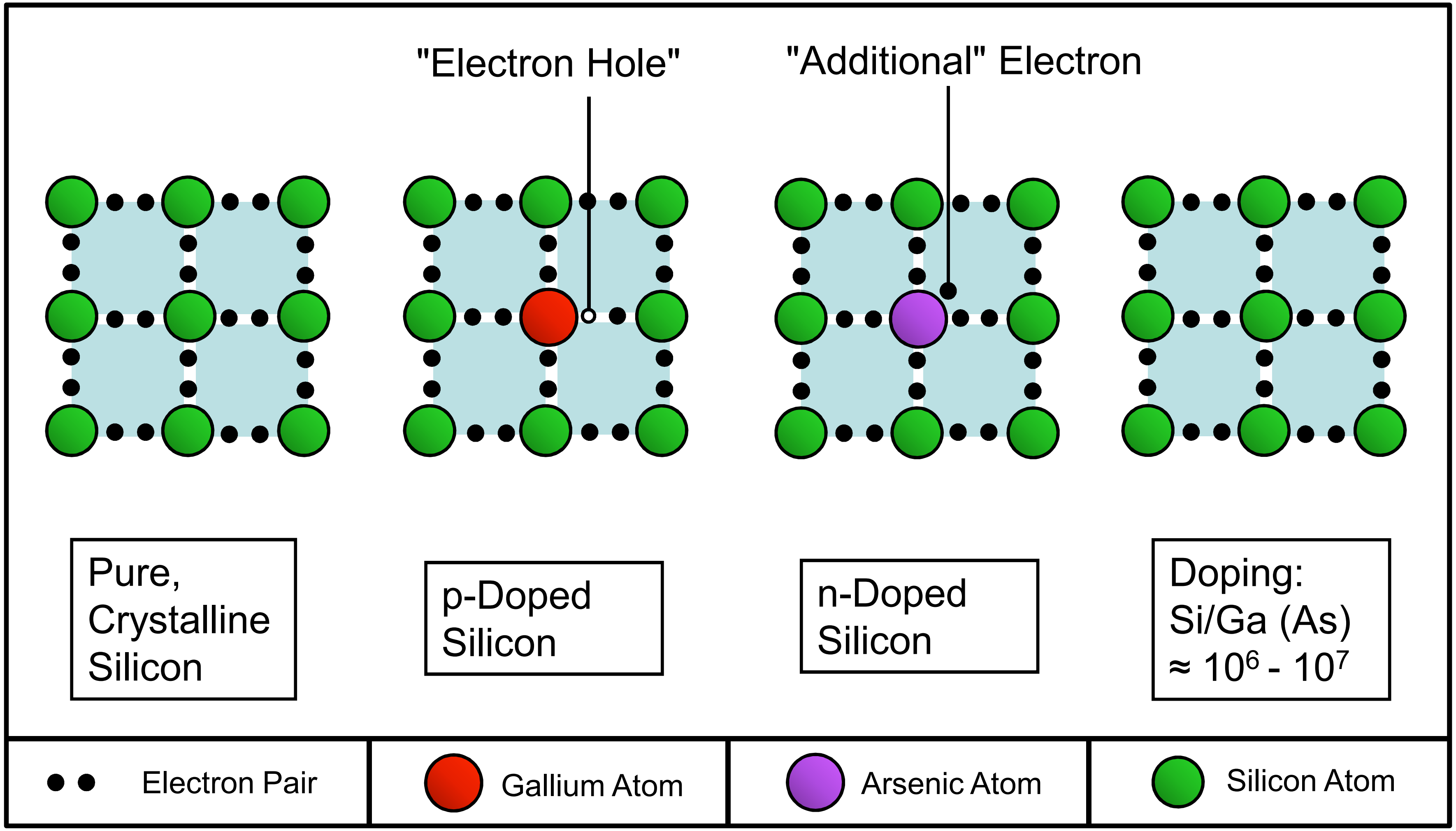
Electrical Properties of Solids; Band Model for Insulators, Metals and Semiconductors.



a) Insulators
b) Metal with only partially occupied lower band: e.g. Lithium (He) $2s^1$. $\rho \approx 10^{-2}\ \Omega\ mm^2m^{-1}$.
c) Metal with overlapping occupied and unoccupied band: e.g. Beryllium (He) $2s^2$.
d) Semiconductor, $\rho \approx 10^5\ \Omega\ mm^2m^{-1}$.

N-Heterocyclic Compounds for OLEDs

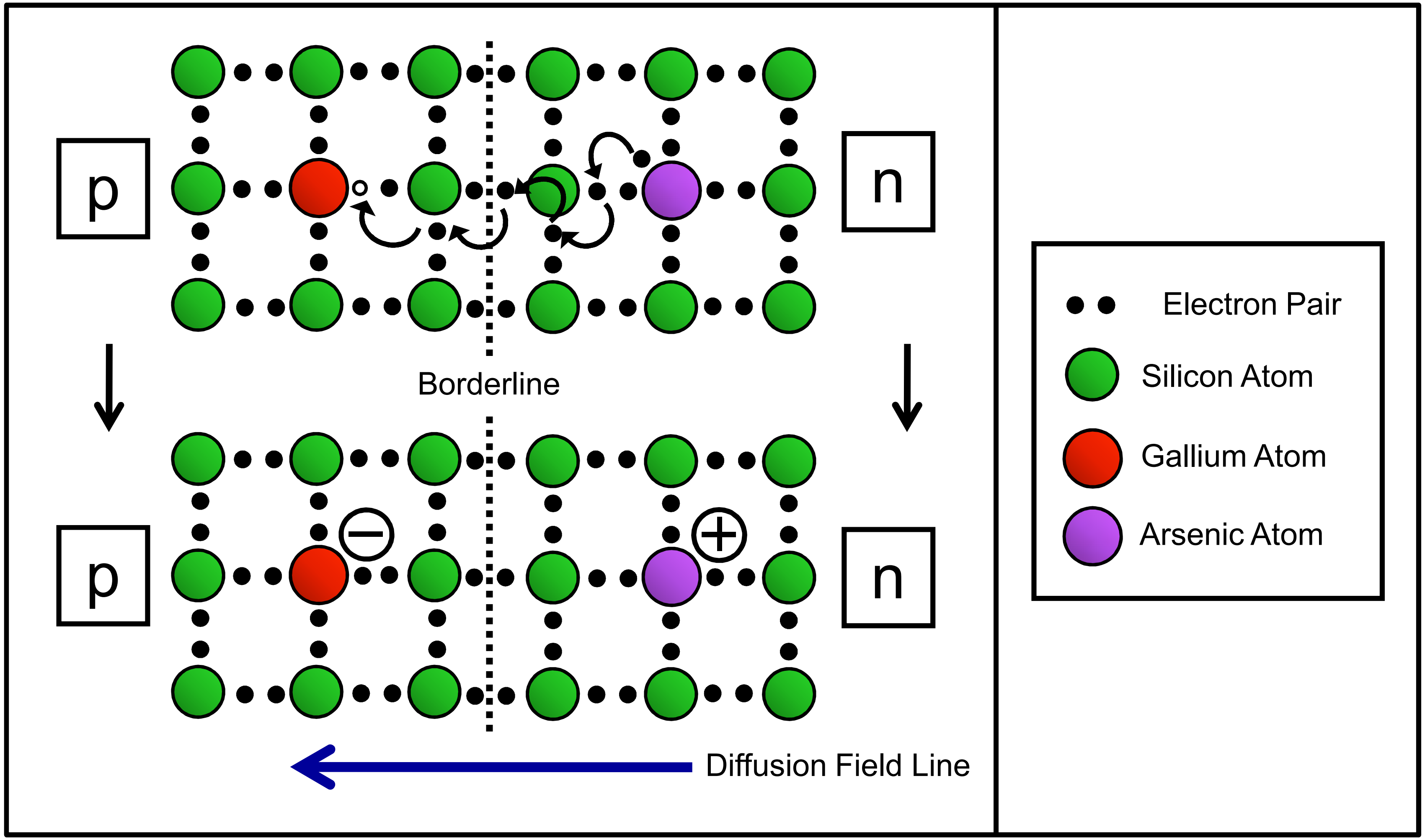
Electrical Properties of Semiconducting Solids
Si-Semiconductors Doped with "Foreign Atoms" as Diode Materials.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

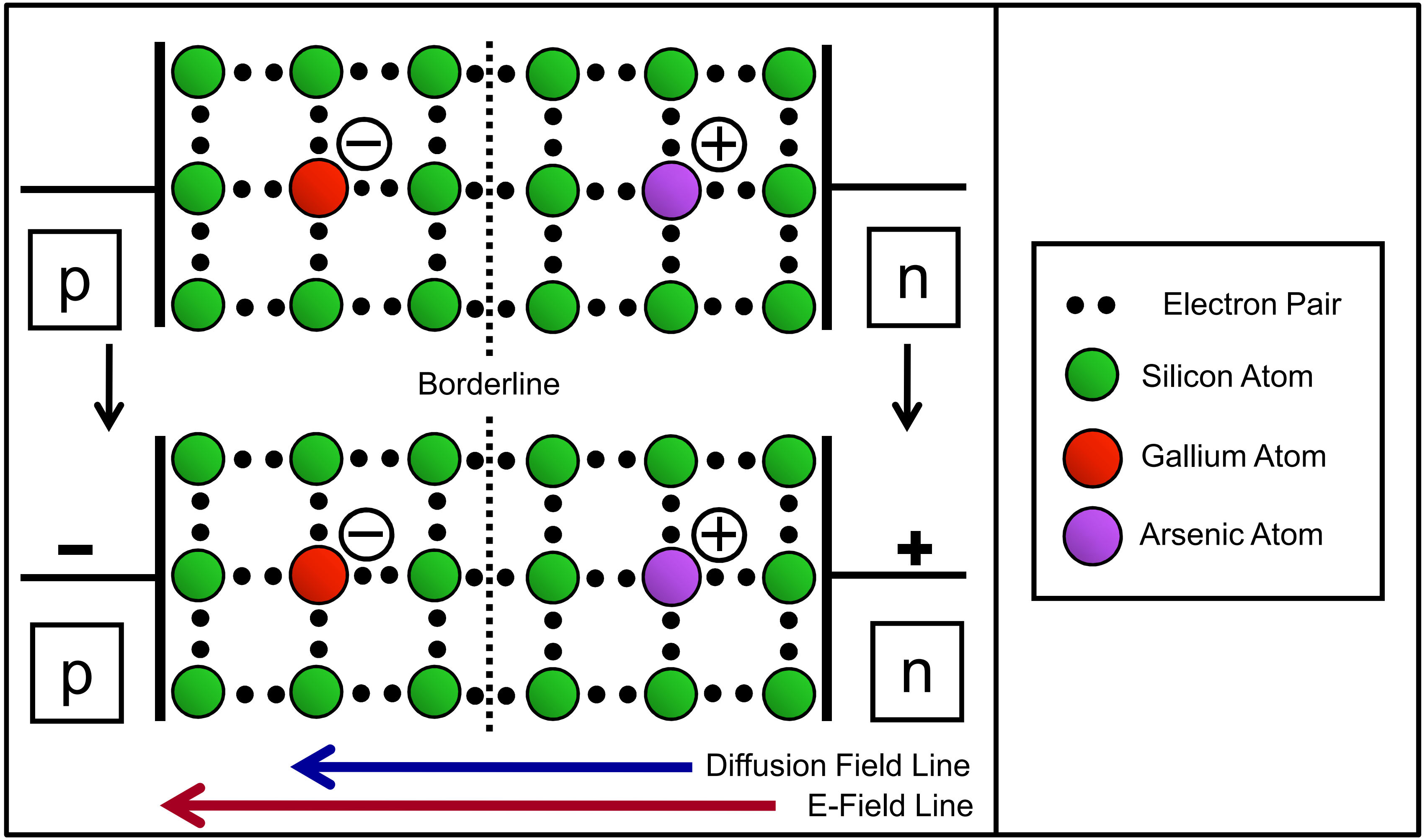
Electron Migration at a pn-Junction: Diffusion Field due to Spontaneous Electrical Charge Separation.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

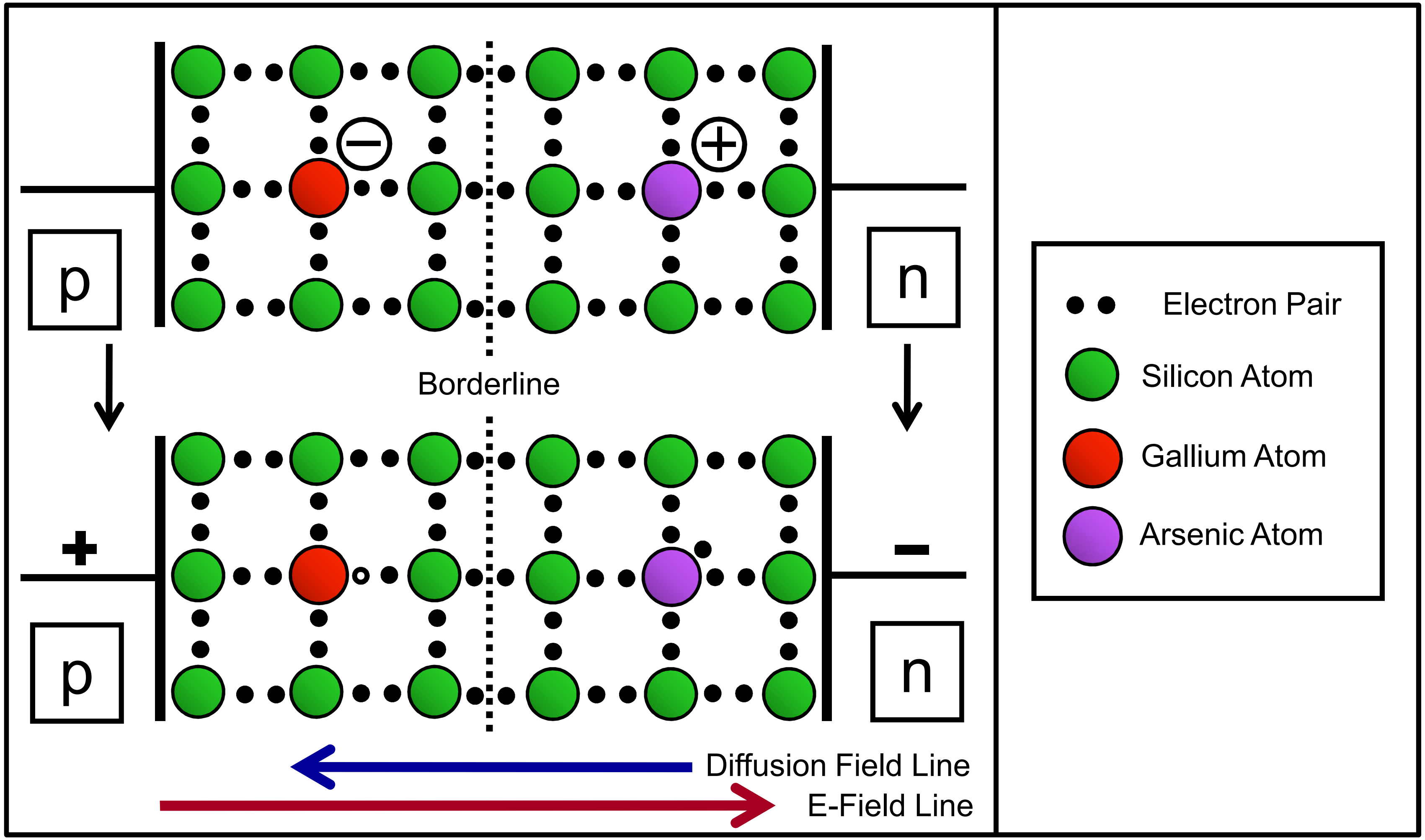
Electron Migration at a pn-Junction: Blocking Case for the Current by Strengthening the Diffusion Field.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

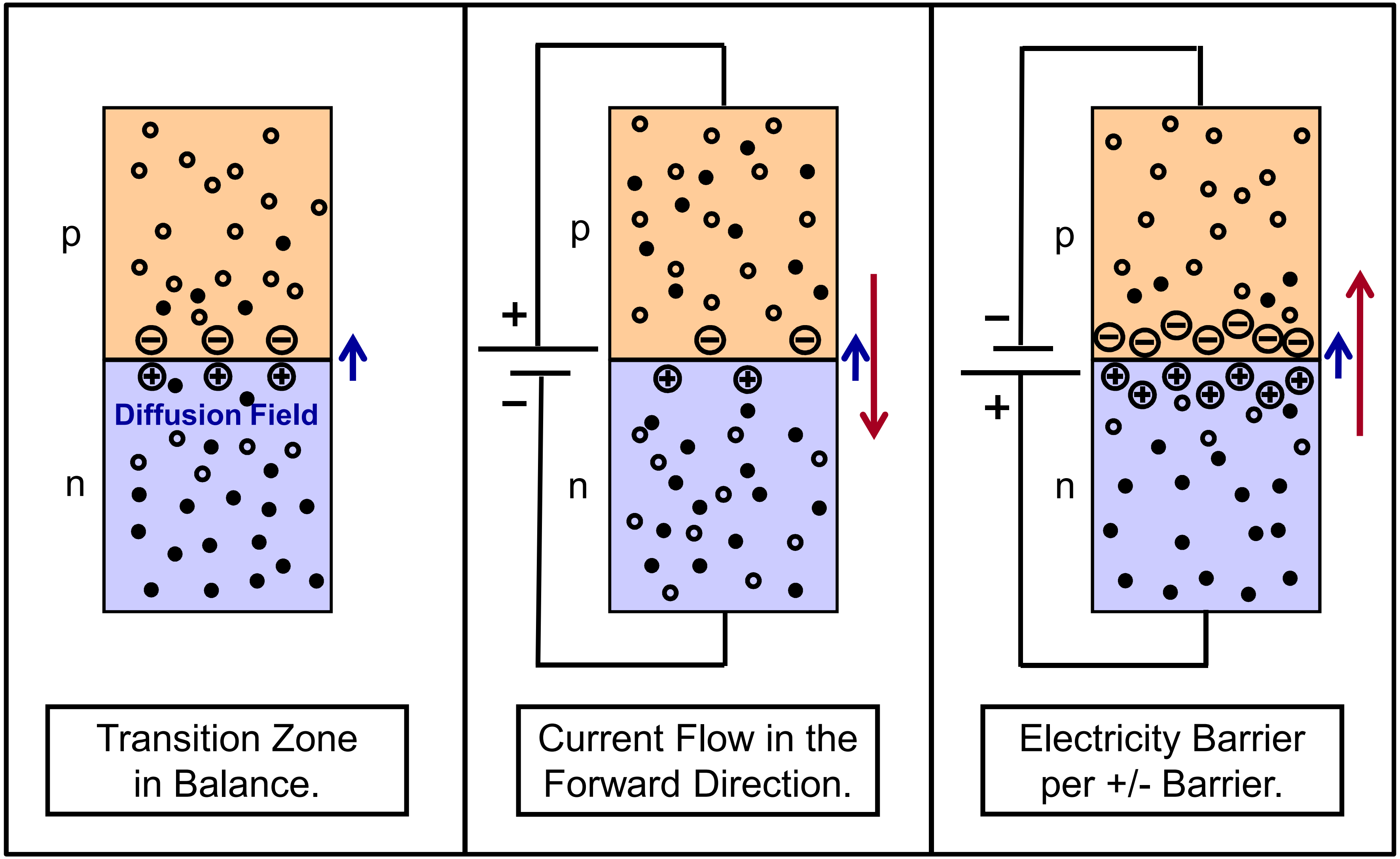
Electron Migration at a pn-Junction:
Current Flow due to Overcompensation of the Diffusion Field.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

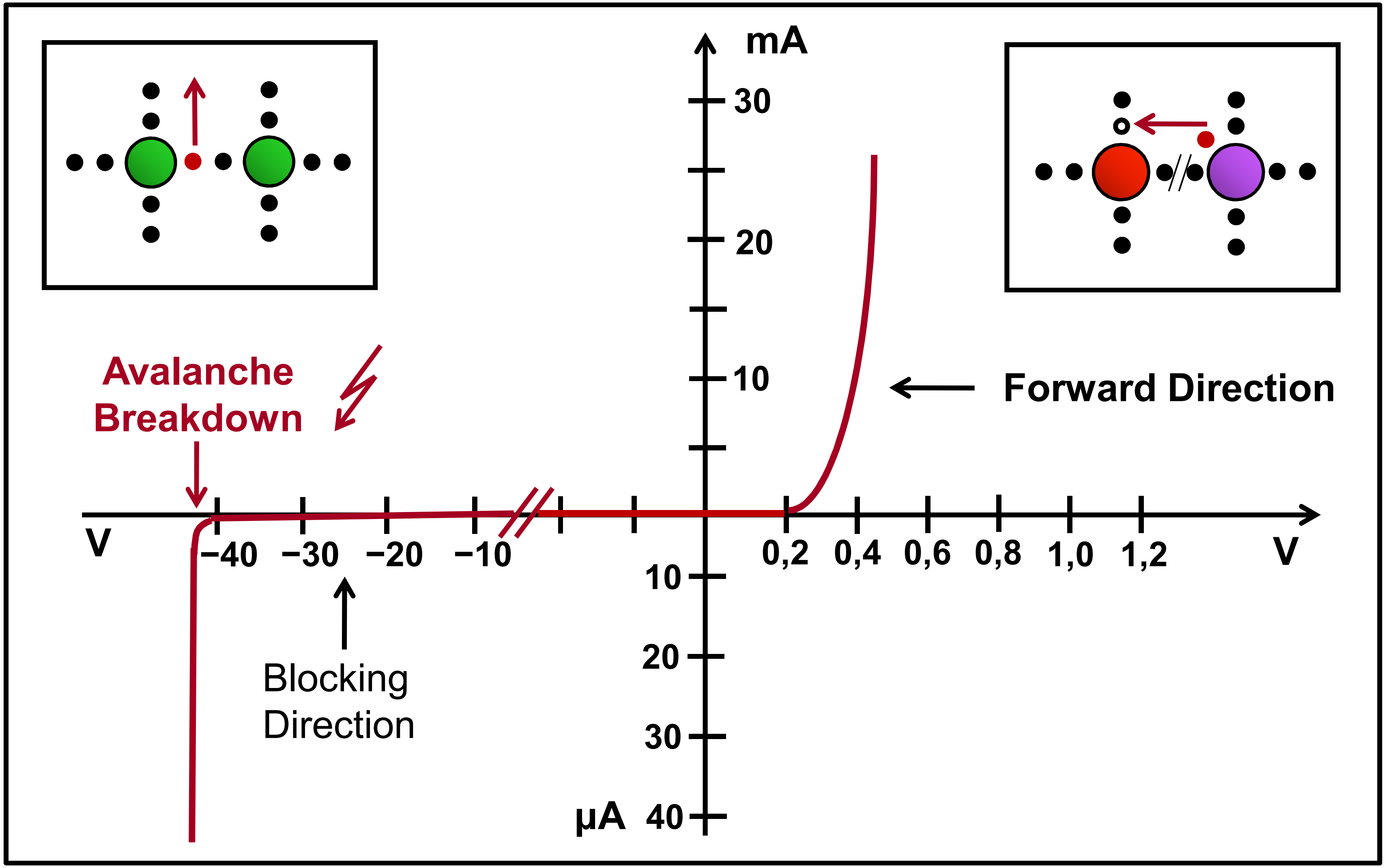
Semiconductor Diode, Function; *Electron:* • *Hole:* ∘



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

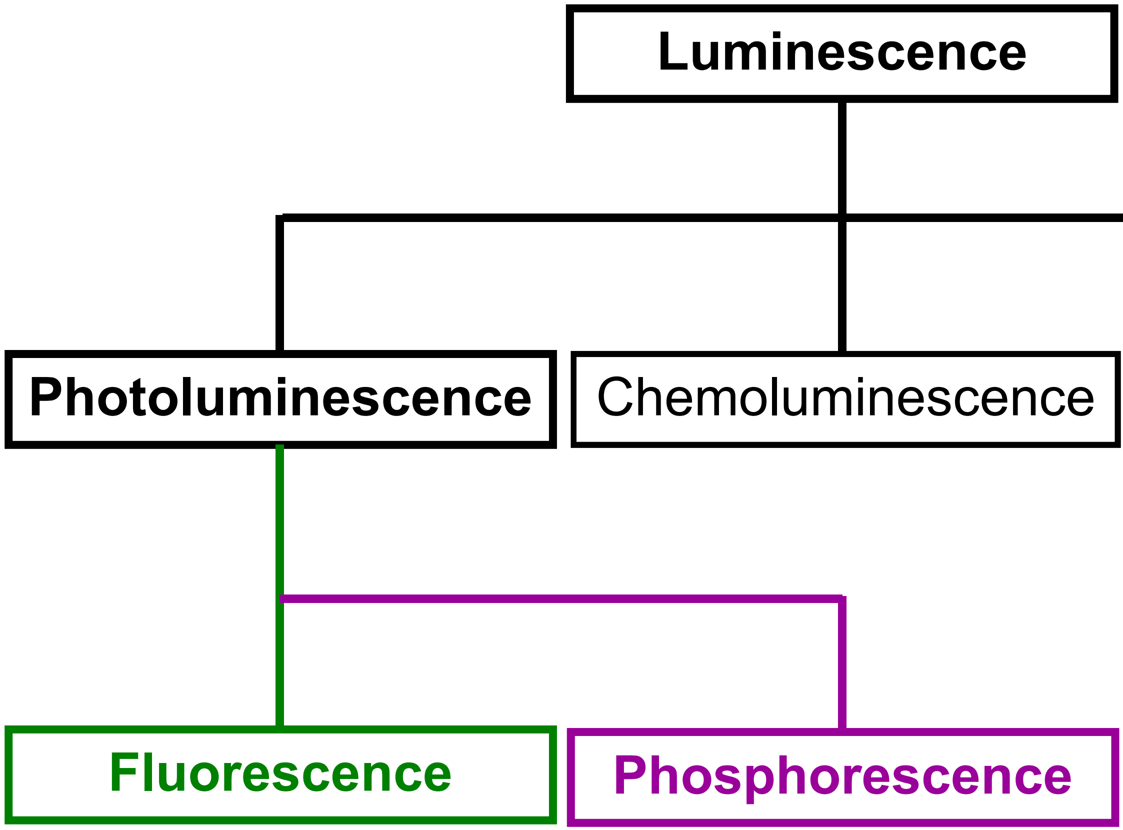
Diode`s Characteristic Curve: Current-Voltage-Chart.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

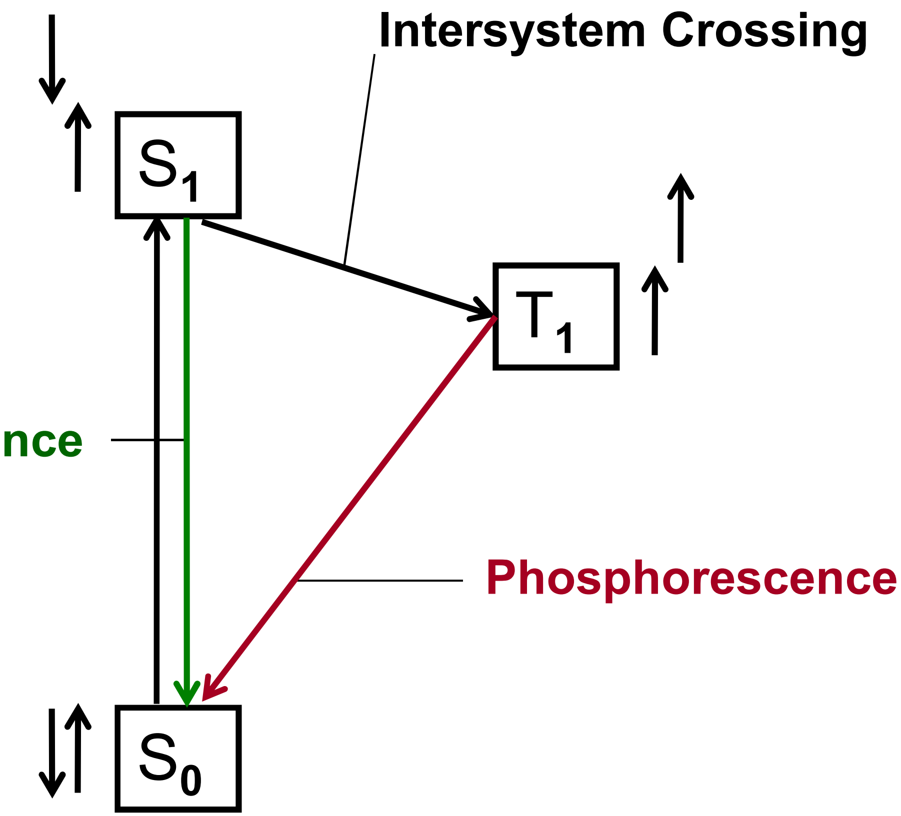
Light Phenomena of Chemical Substances:



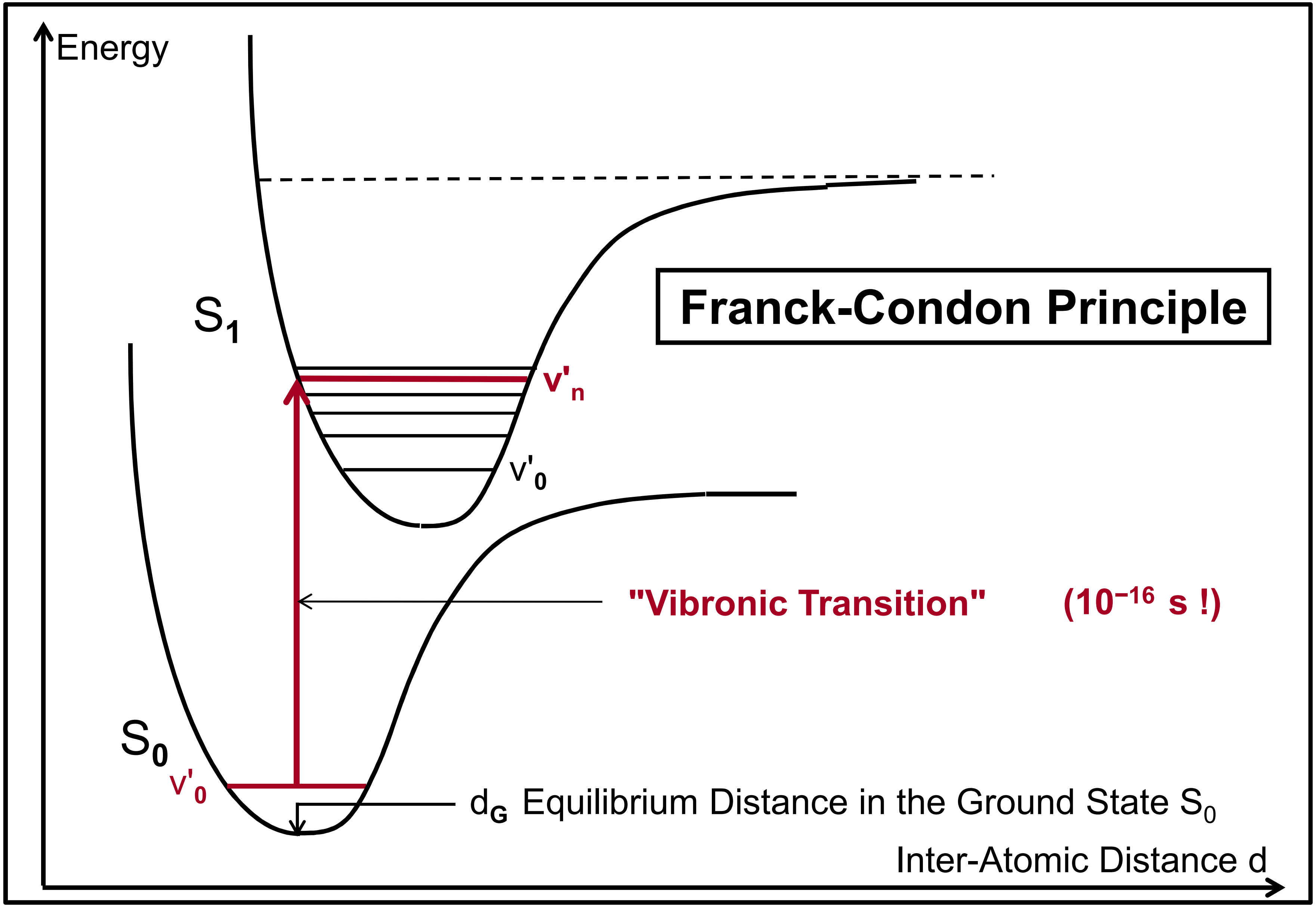
Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

Fluorescence and Phosphorescence:

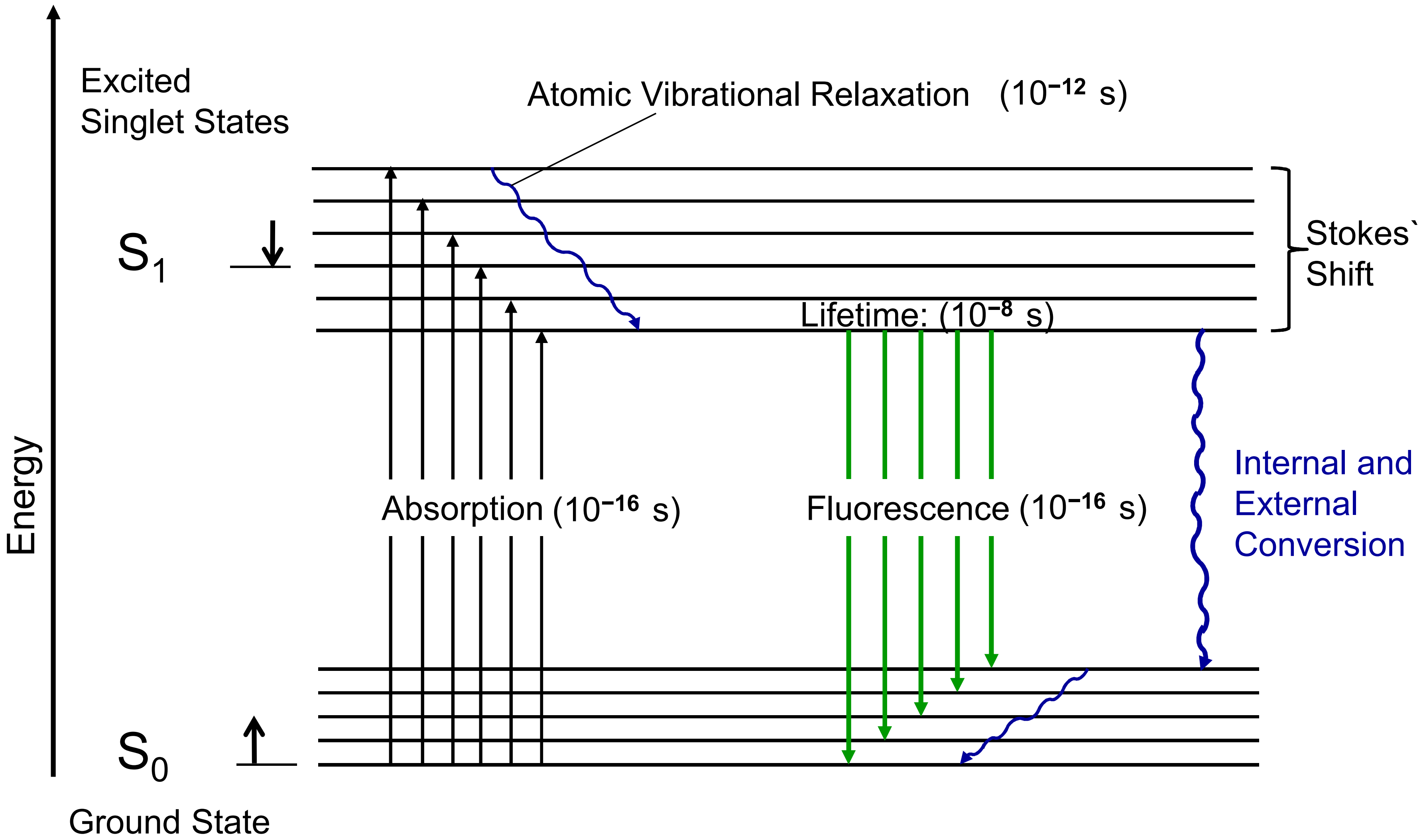


N-Heterocyclic Compounds for OLEDs



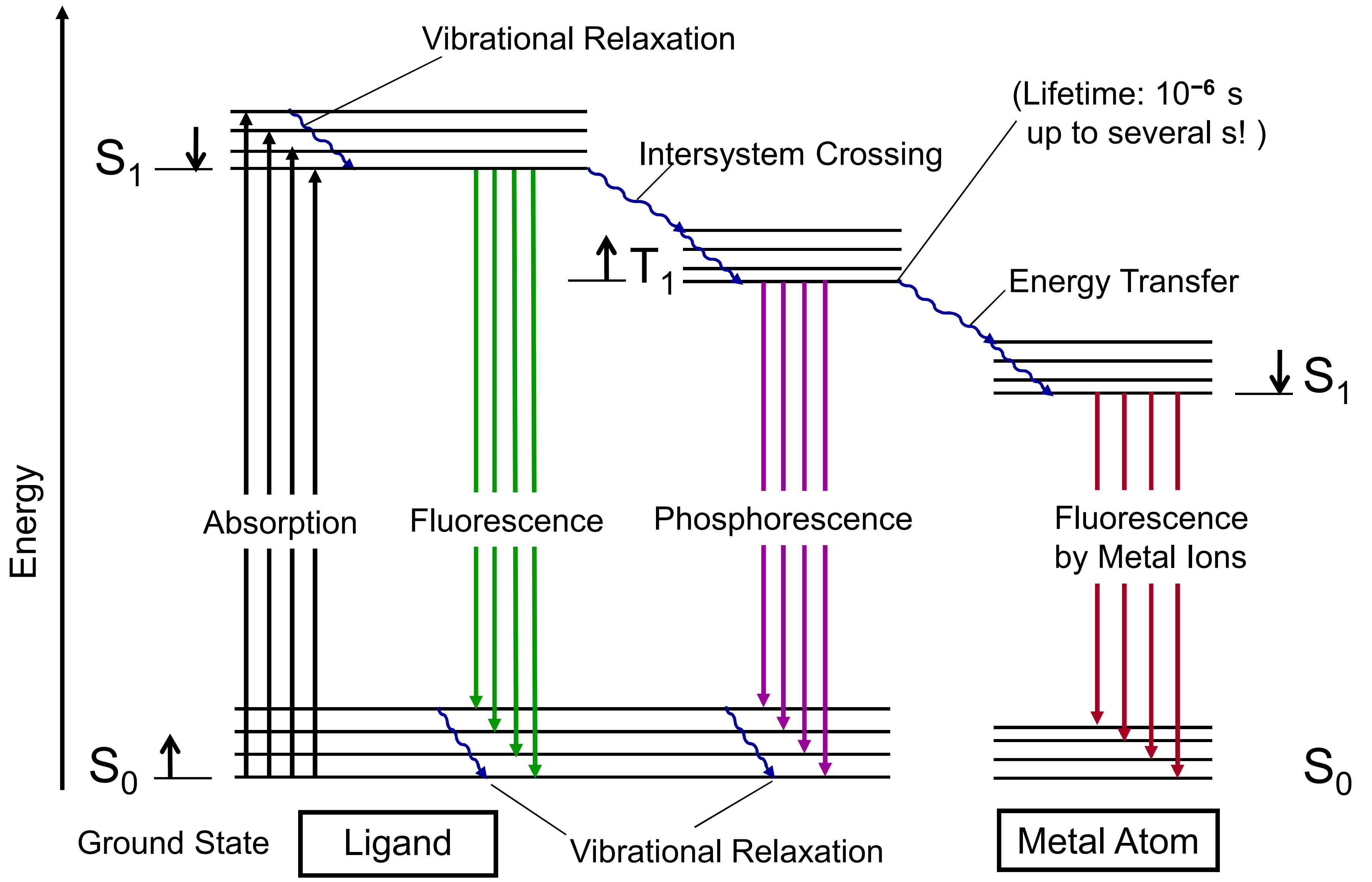
N-Heterocyclic Compounds for OLEDs

Jablonski-Diagram for the Fluorescence:



Jablonski–Diagram

"Time-Delayed Fluorescence" of Metal Chelates:

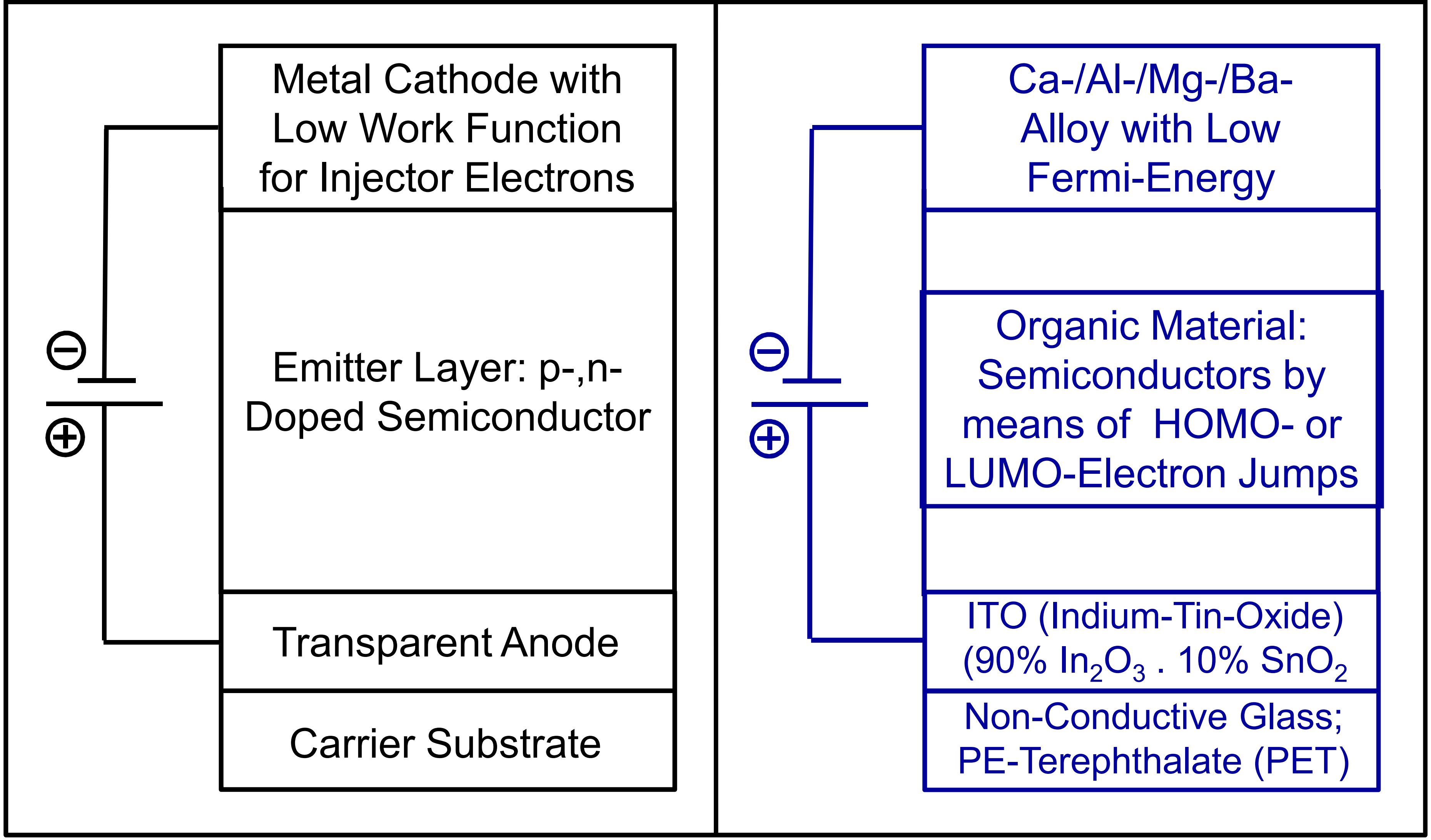


Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

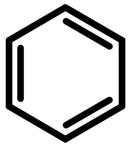
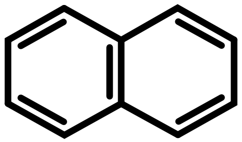
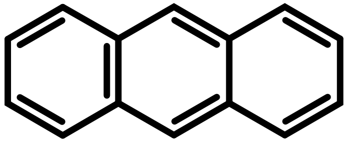
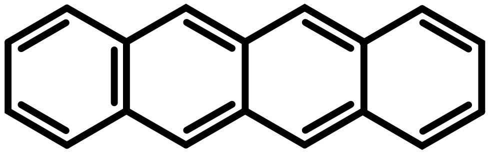
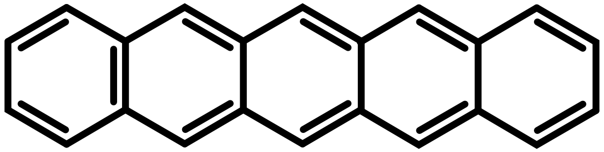
OLED, Organic Light Emitting Diode

Structure of a Single Layer-LED or -OLED, "Sandwich-Structures" :



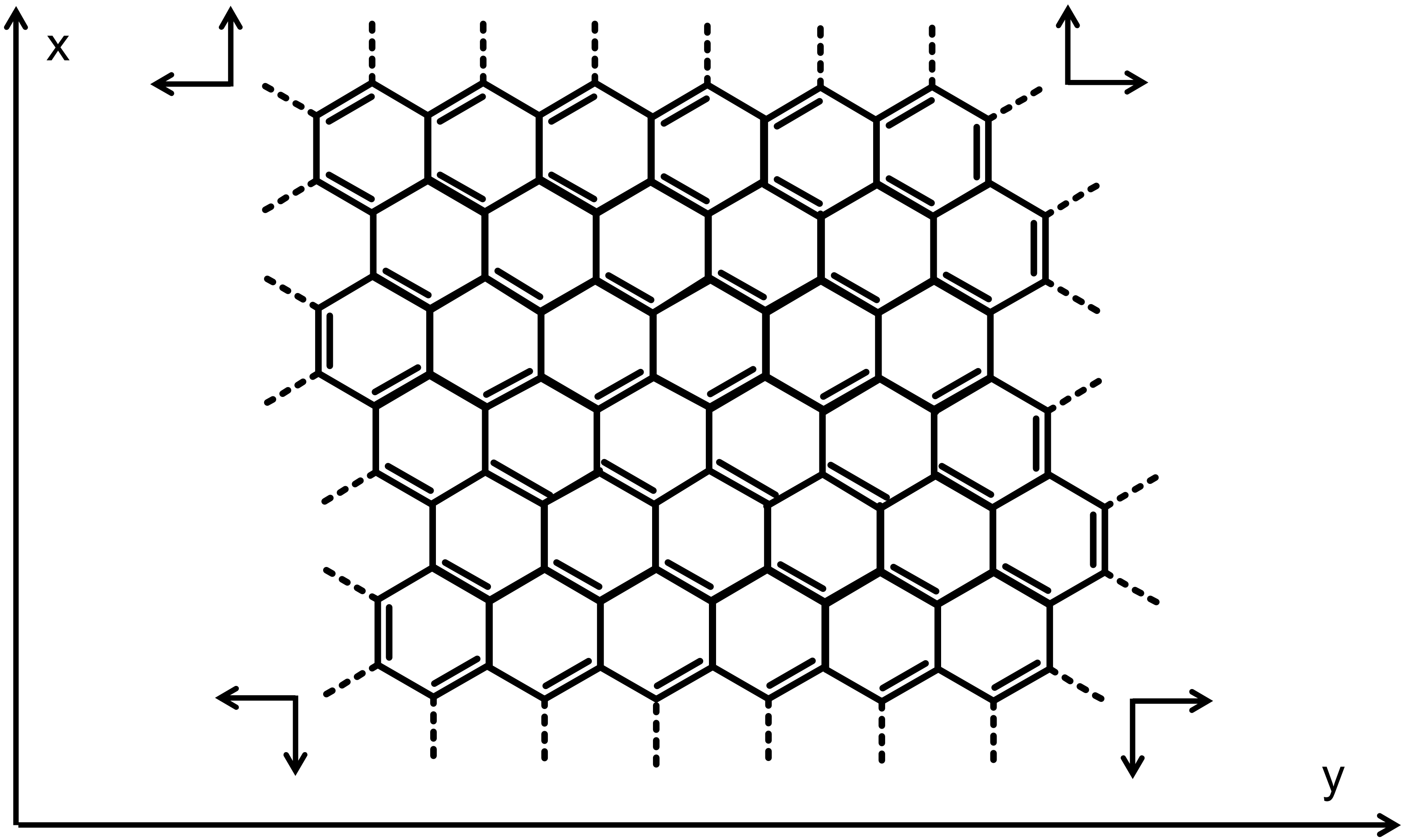
N-Heterocyclic Compounds for OLEDs

Conjugation of Aromatic Hydrocarbons, HOMO-LUMO-Distances and Fluorescence Wavelengths.

		$S_1 \approx$ 6,0 eV	200 nm	Benzene
		$S_1 \approx$ 4,3 eV	290 nm	Naphtalene
		$S_1 \approx$ 3,3 eV	380 nm	Anthracene
		$S_1 \approx$ 2,4 eV	525 nm	Tetracene
		$S_1 \approx$ 2,1 eV	580 nm	Pentacene

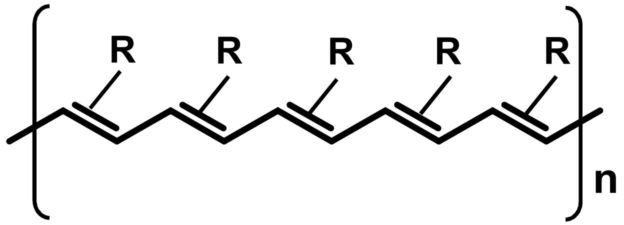
Rainer Buerstinghaus

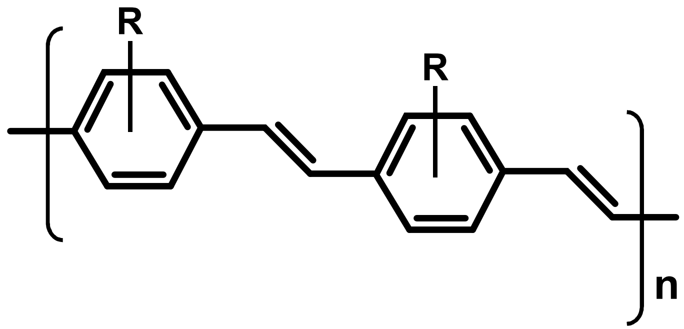
π-Conjugation of Graphene (Detail) as a Conductor.

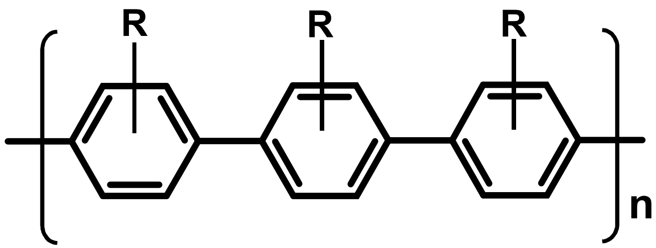


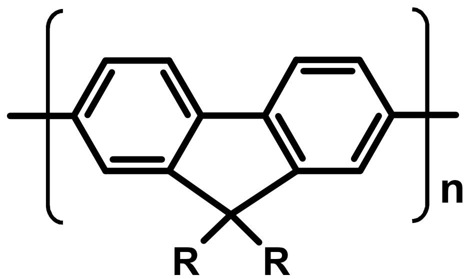
N-Heterocyclic Compounds for OLEDs

OLED, Conjugated Polymers as Organic Semiconductors.





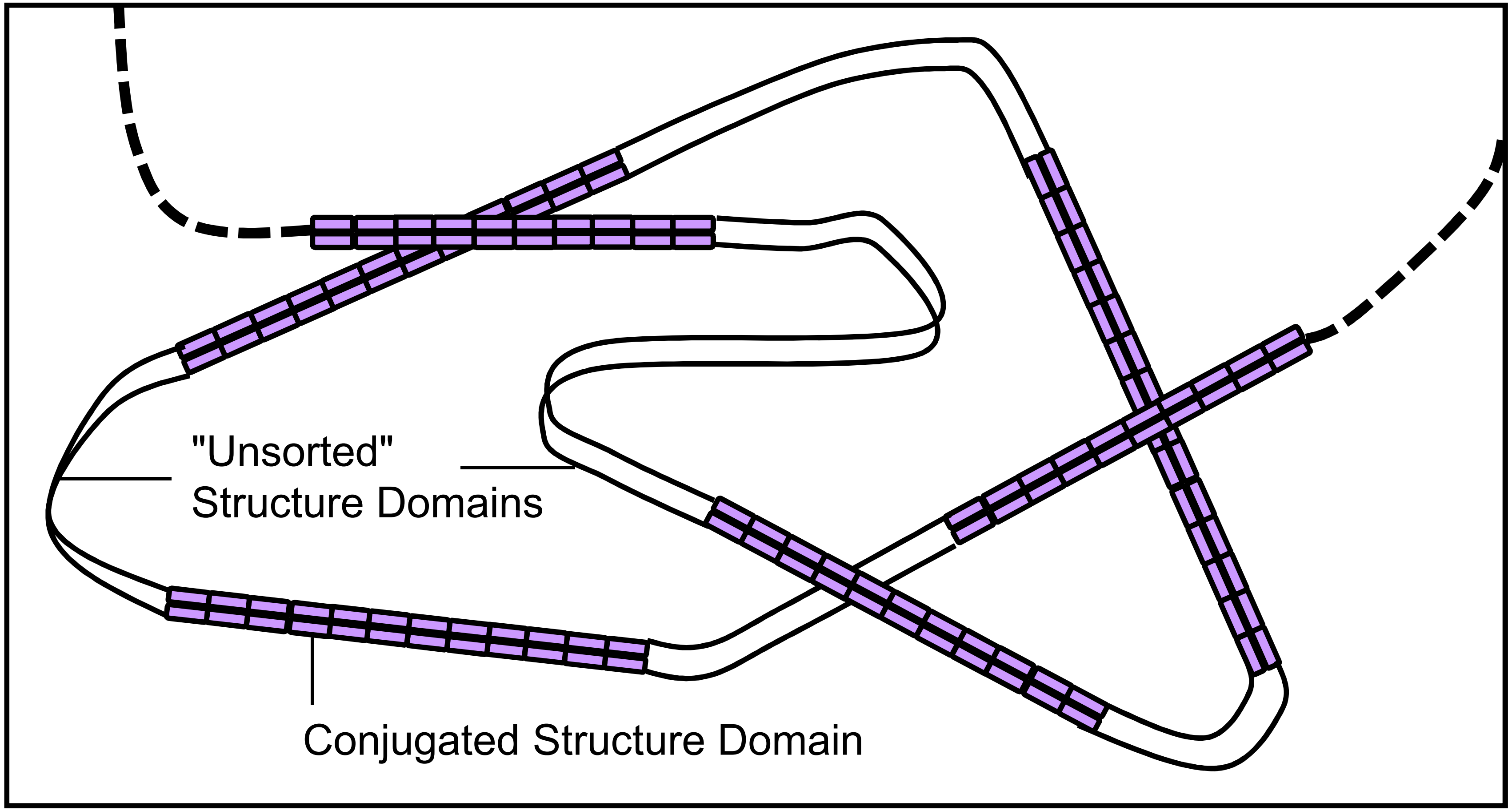




Rainer Buerstinghaus

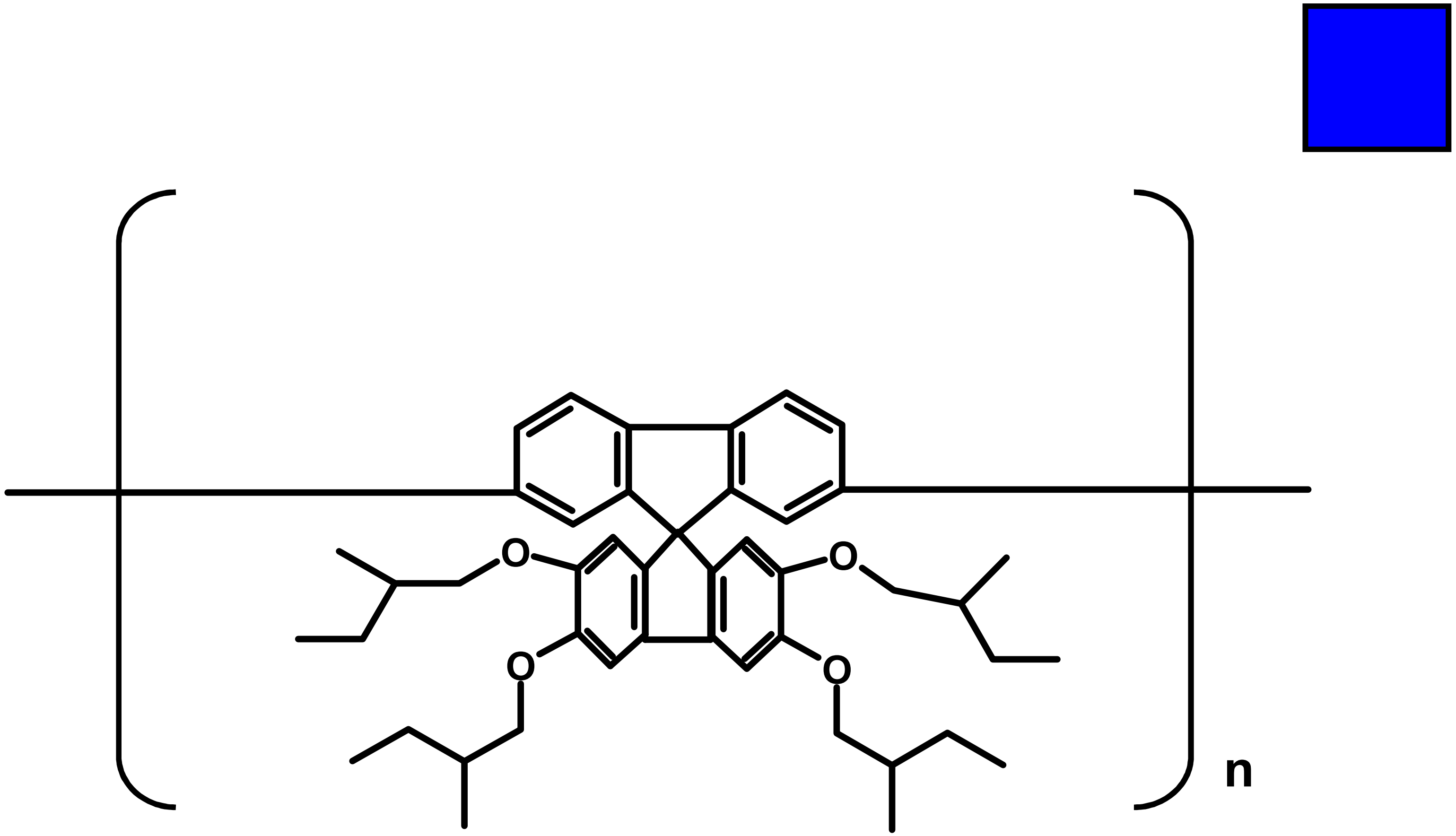
N-Heterocyclic Compounds for OLEDs

OLEDs: Conjugated Polymers as Semiconductors.
Effective Conjugation Length ≈ 6nm ≈ 10-15 Monomer Units.
Causes: Kinks, Defects, Twists. Application: Via Spin Coating.

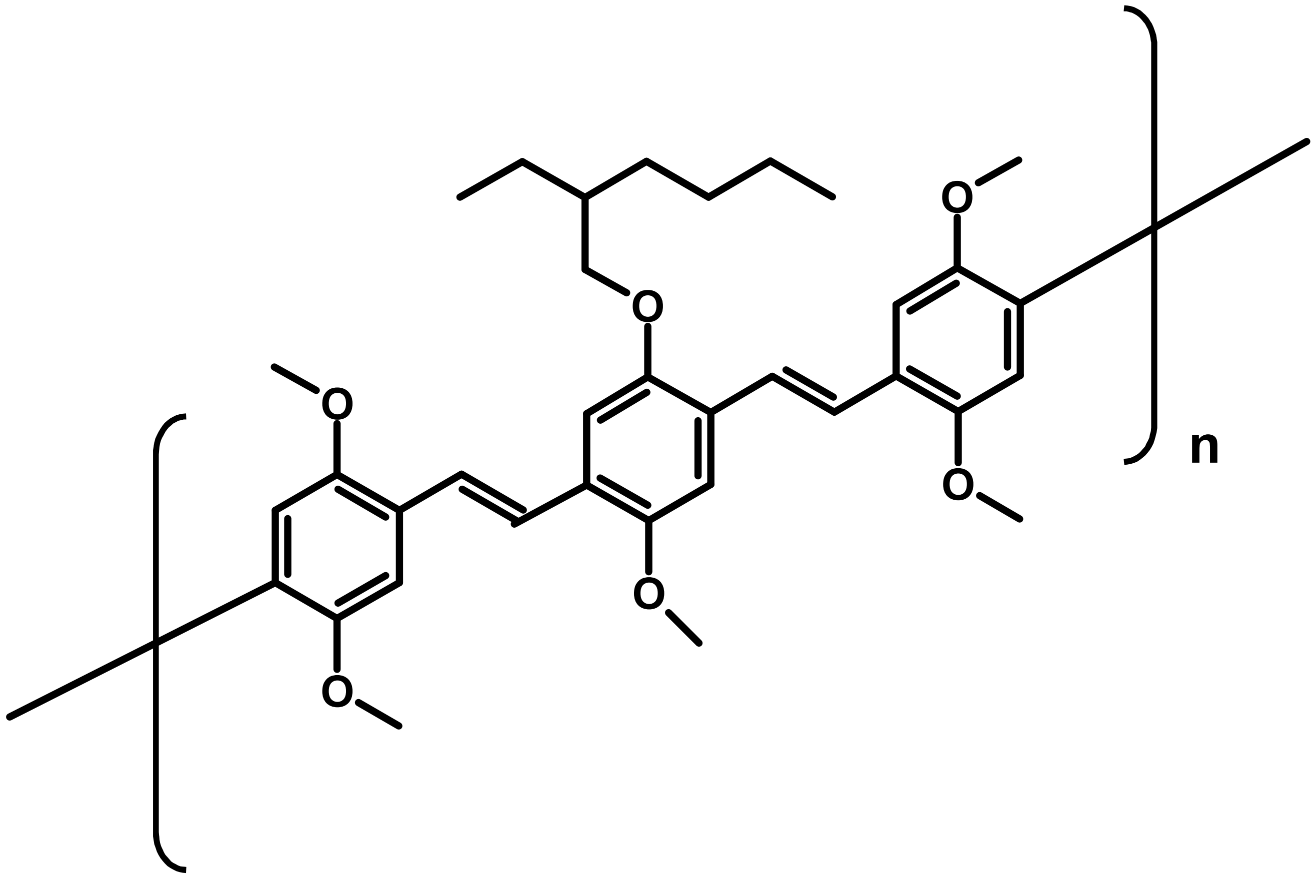


Rainer Buerstinghaus

OLED, Electroluminescent Polymers: Blue.

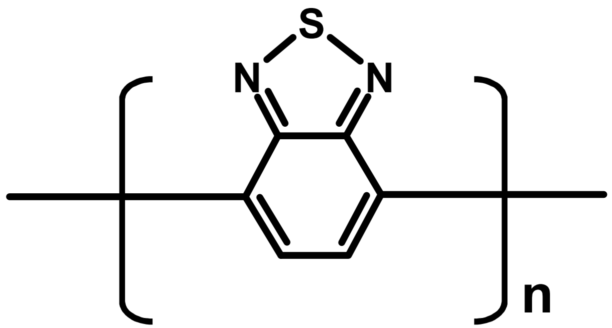


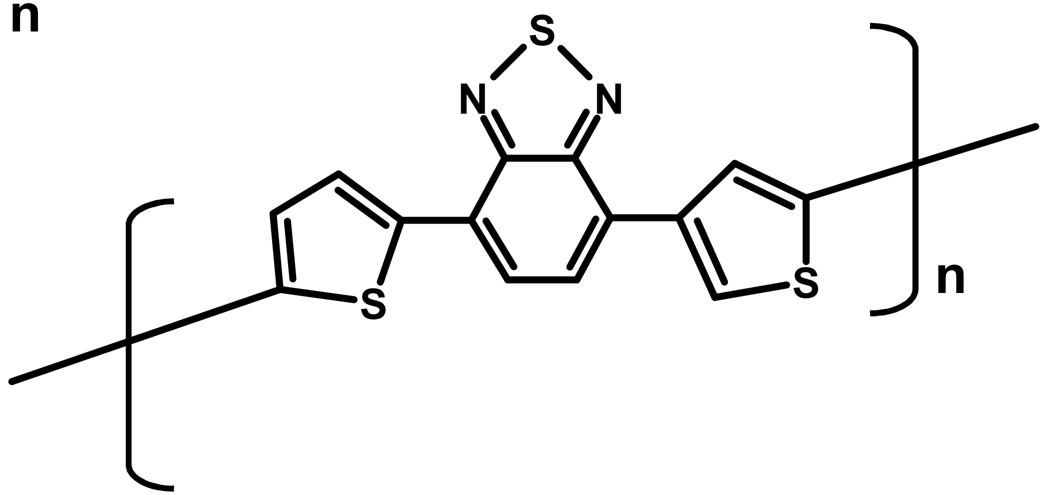
OLED, Electroluminescent Polymers: Green.



Rainer Buerstinghaus

OLED, Electroluminescent Polymers: Red.



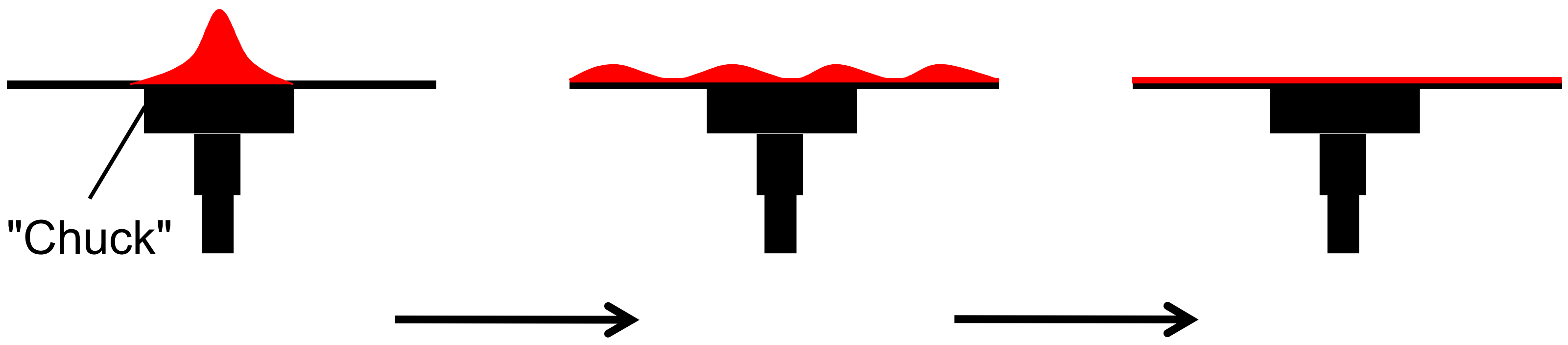


Spin Coating Process, Schematic Representation.

Application of 1-3 ml of a solution of the unsat. Polymer.

Evaporation of the solvent, increase in viscosity.

Removal of the polymer solution (Approxim. 90%).



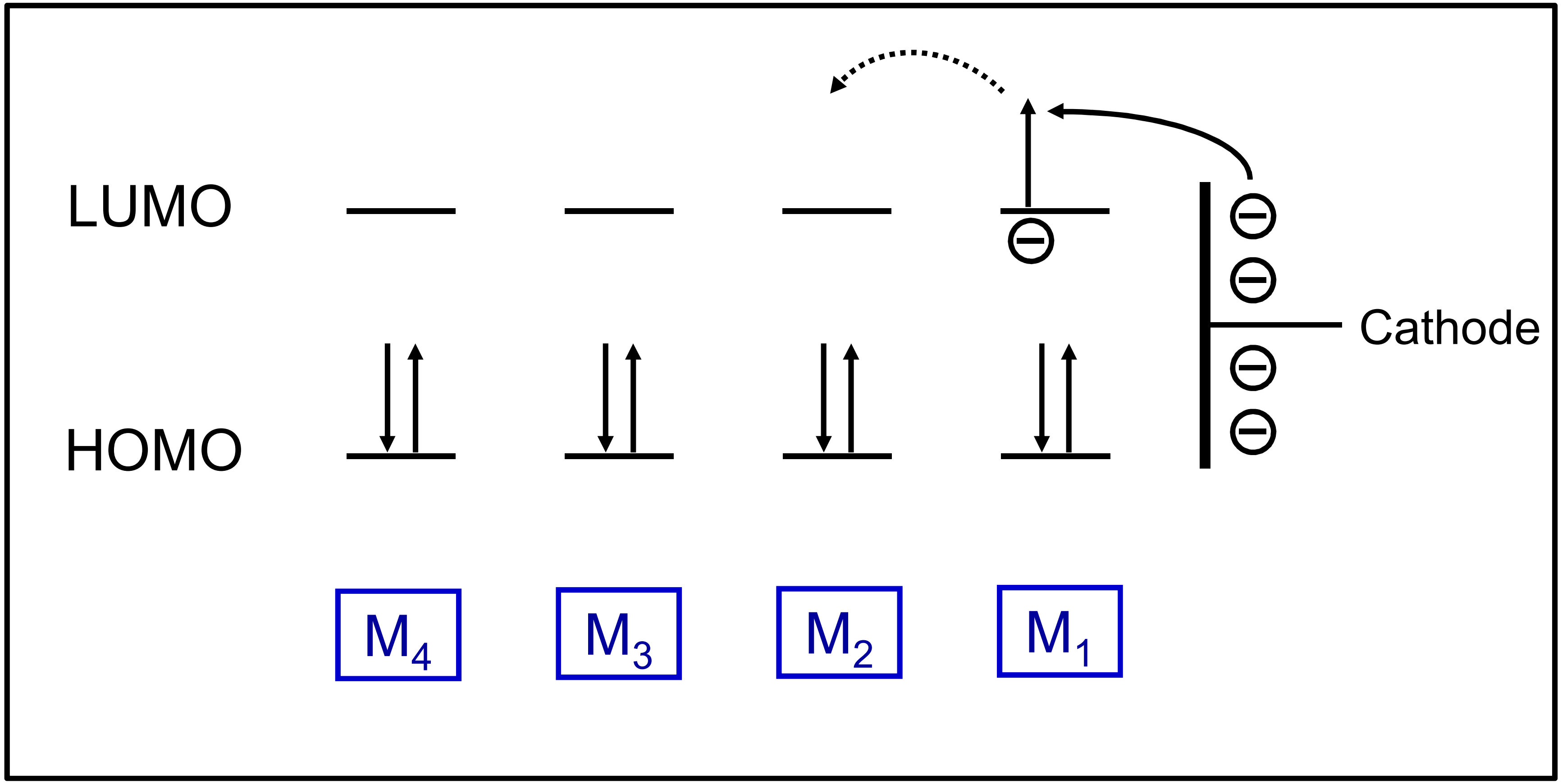
Forming
(Low Rotation Number, ≈ 500 Revolutions/Minute)

Centrifugation
(Higher Rotation Number, ≈ 5.000 Revolutions/Minute)

Rainer Buerstinghaus

Electron Transport Between Semiconducting Molecules.

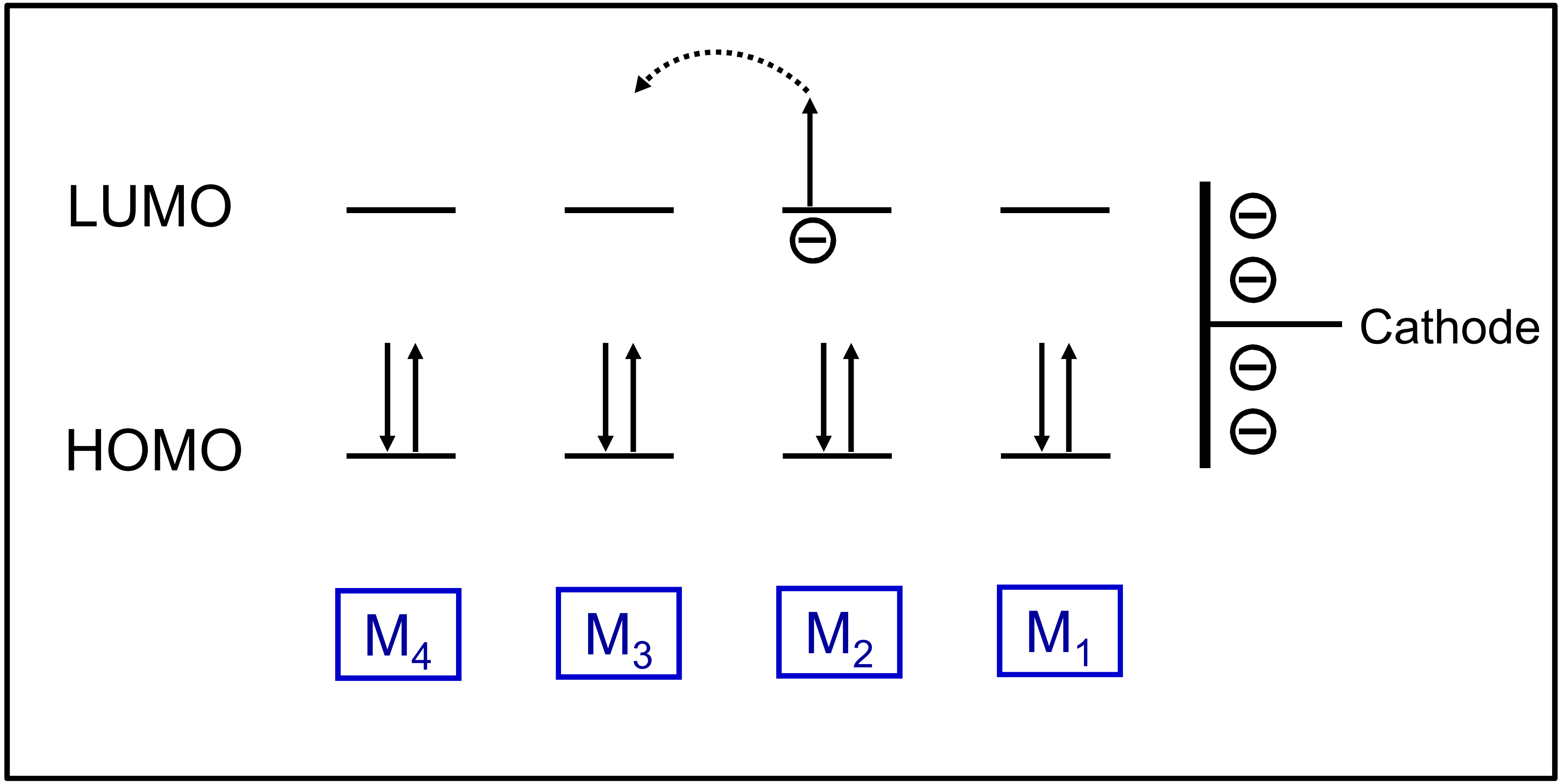
HOMO: Highest Occupied Molecular Orbital
LUMO: Lowest Unoccupied Molecular Orbital



N-Heterocyclic Compounds for OLEDs

Electron Transport Between Semiconducting Molecules.

HOMO: Highest Occupied Molecular Orbital
LUMO: Lowest Unoccupied Molecular Orbital

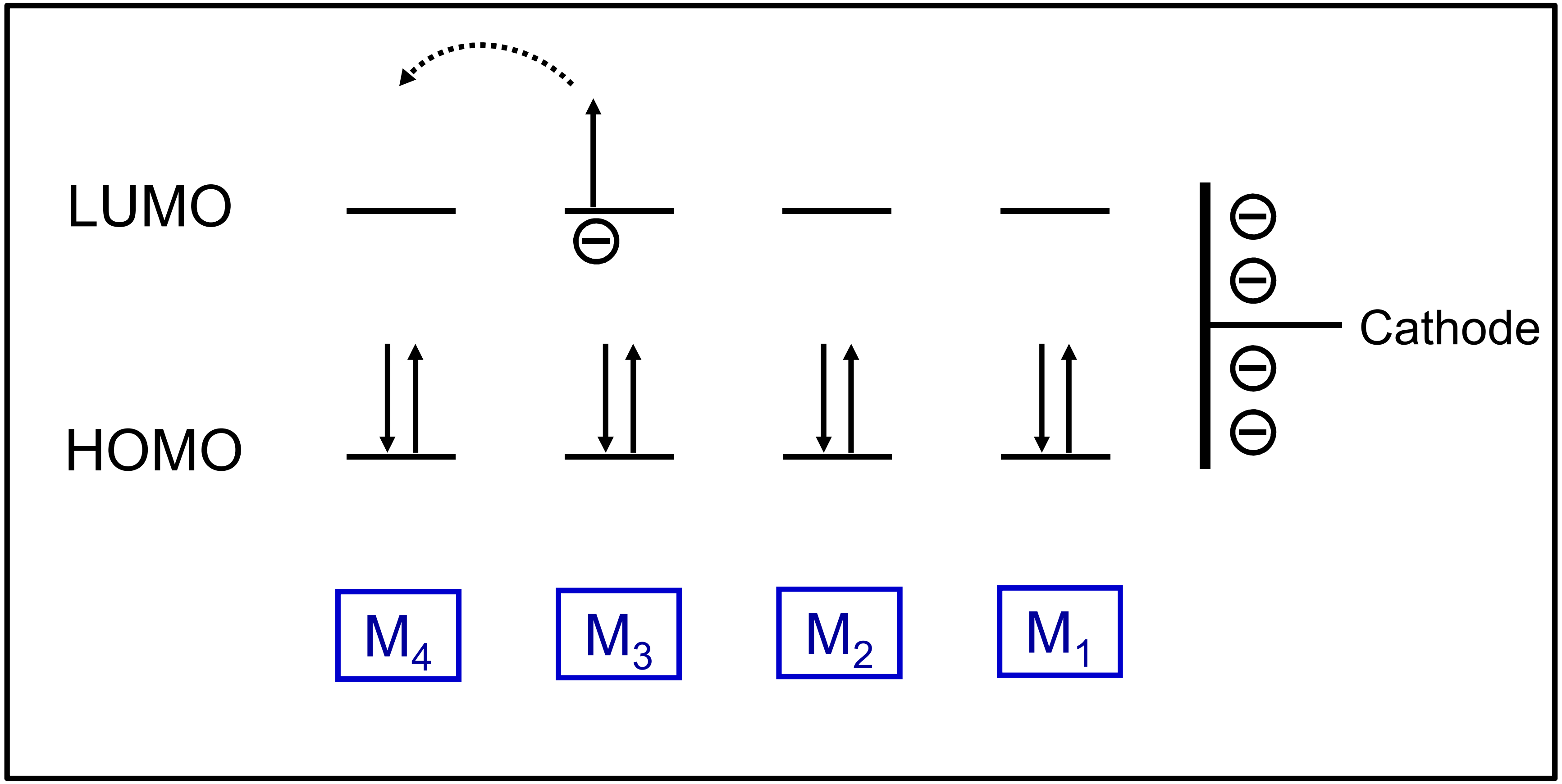


Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

Electron Transport Between Semiconducting Molecules.

HOMO: Highest Occupied Molecular Orbital
LUMO: Lowest Unoccupied Molecular Orbital

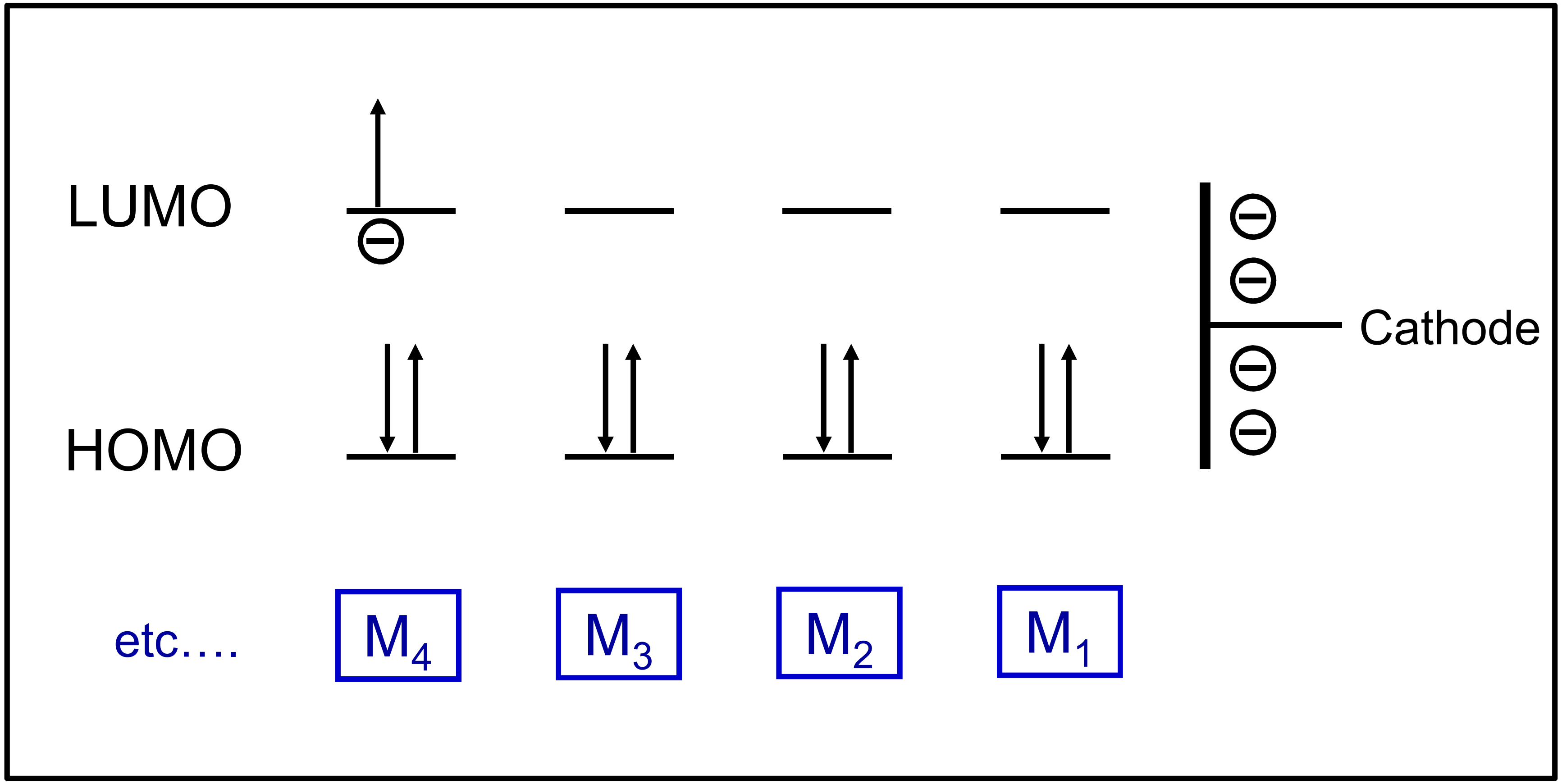


Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

Electron Transport Between Semiconducting Molecules.

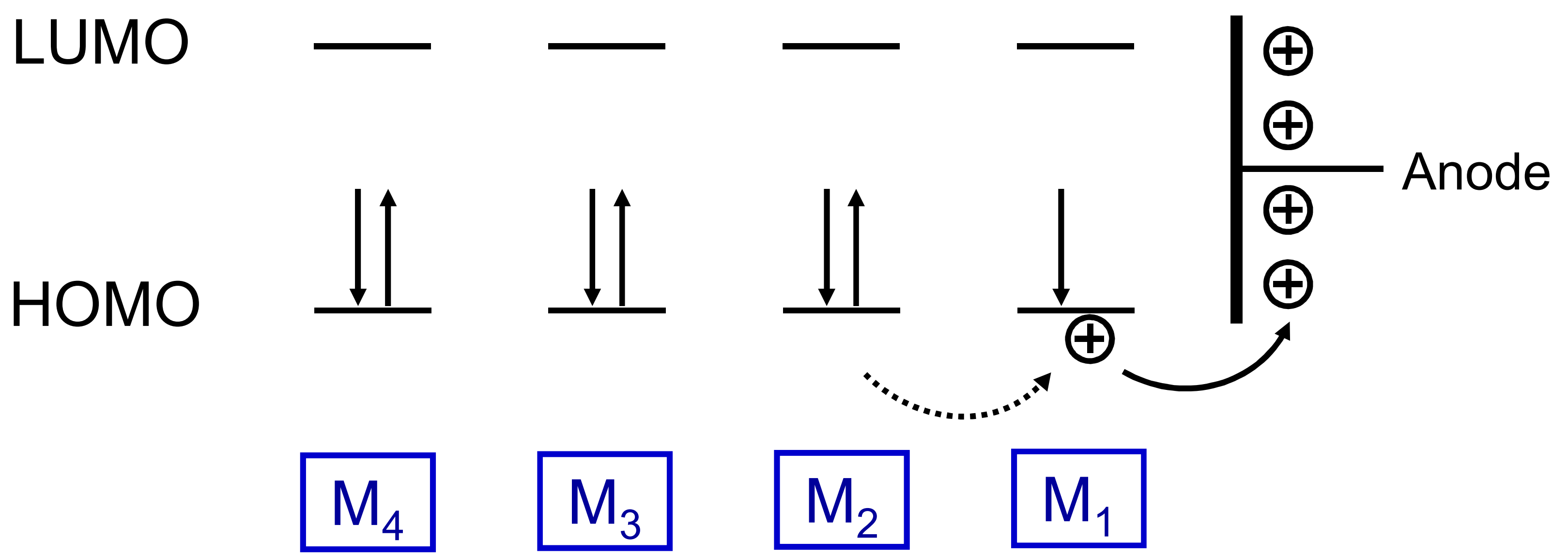
HOMO: Highest Occupied Molecular Orbital
LUMO: Lowest Unoccupied Molecular Orbital



Rainer Buerstinghaus

Electron Transport Between Semiconducting Molecules.

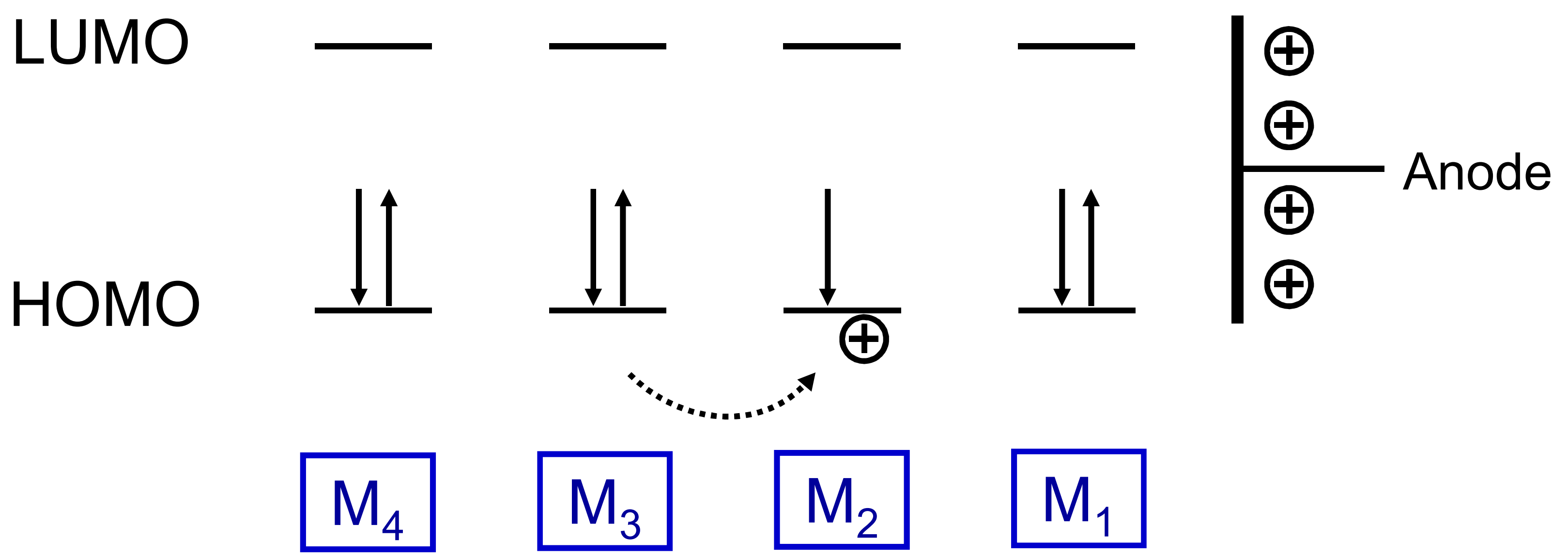
HOMO: Highest Occupied Molecular Orbital
LUMO: Lowest Unoccupied Molecular Orbital



Rainer Buerstinghaus

Electron Transport Between Semiconducting Molecules.

HOMO: Highest Occupied Molecular Orbital
LUMO: Lowest Unoccupied Molecular Orbital

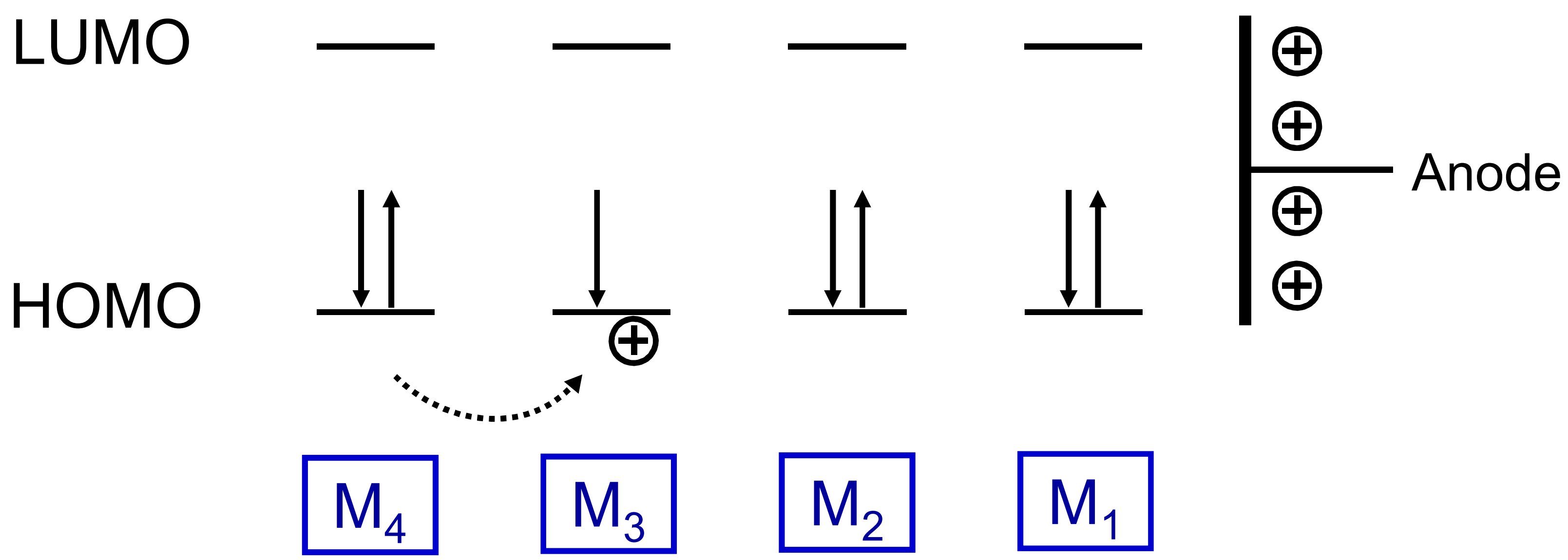


Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

Electron Transport Between Semiconducting Molecules.

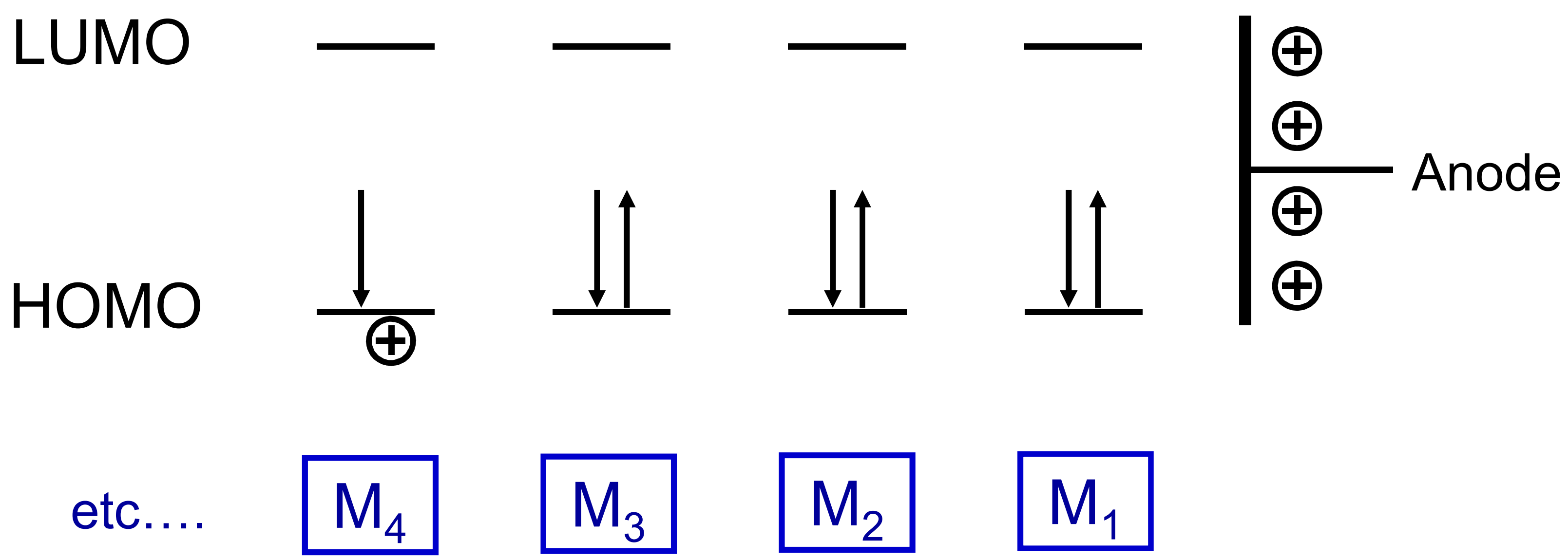
HOMO: Highest Occupied Molecular Orbital
LUMO: Lowest Unoccupied Molecular Orbital



N-Heterocyclic Compounds for OLEDs

Electron Transport Between Semiconducting Molecules.

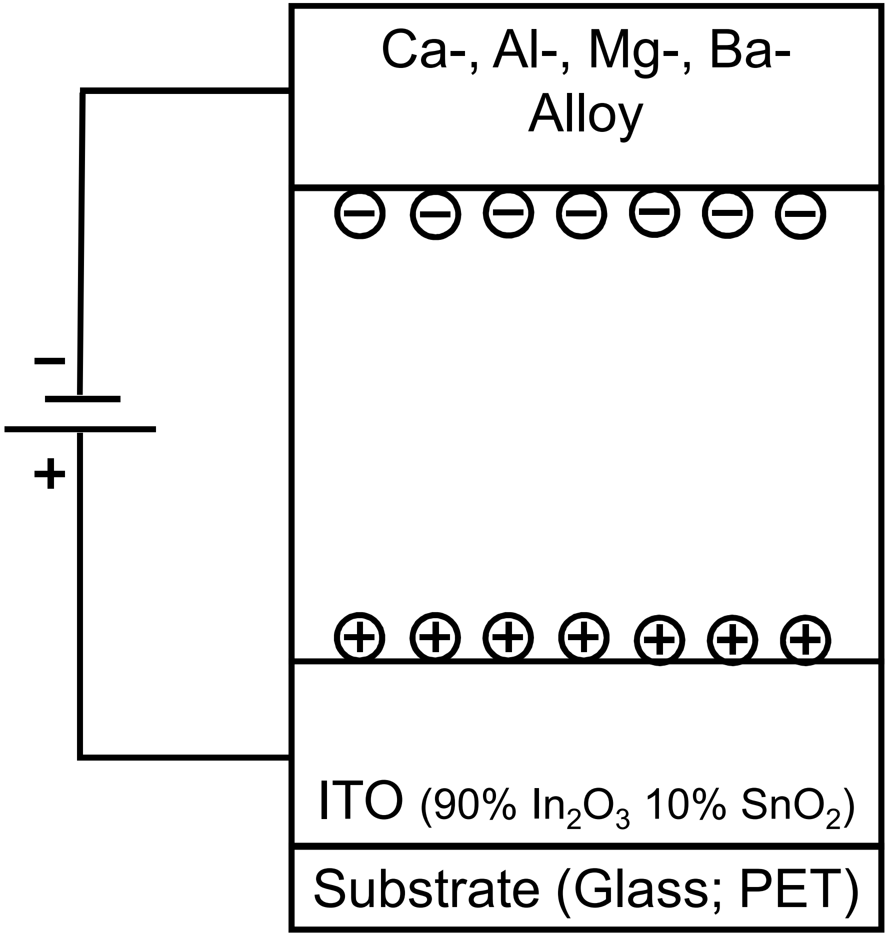
HOMO: Highest Occupied Molecular Orbital
LUMO: Lowest Unoccupied Molecular Orbital



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

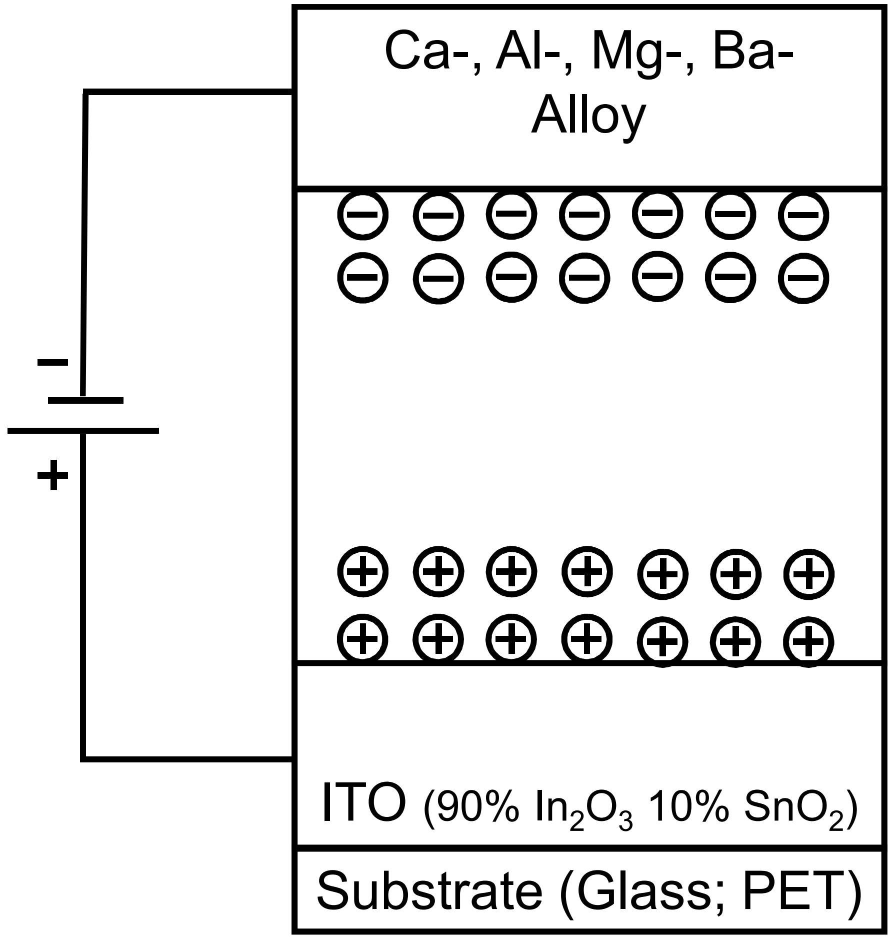
OLED, **O**rganic **L**ight **E**mitting **D**iode, **Single Layer–OLED.**



Start of the Electron-Hole Migration.

N-Heterocyclic Compounds for OLEDs

OLED, **O**rganic **L**ight **E**mitting **D**iode, **Single Layer–OLED.**

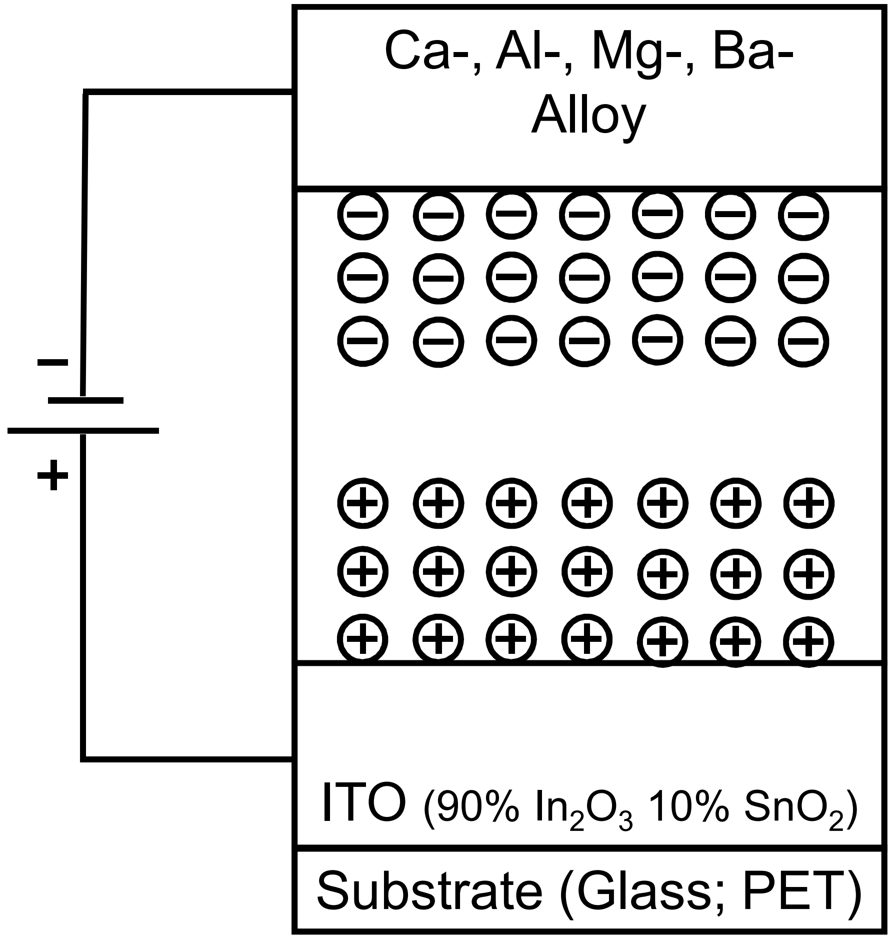


Progression of the Electron-Hole Migration.

Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

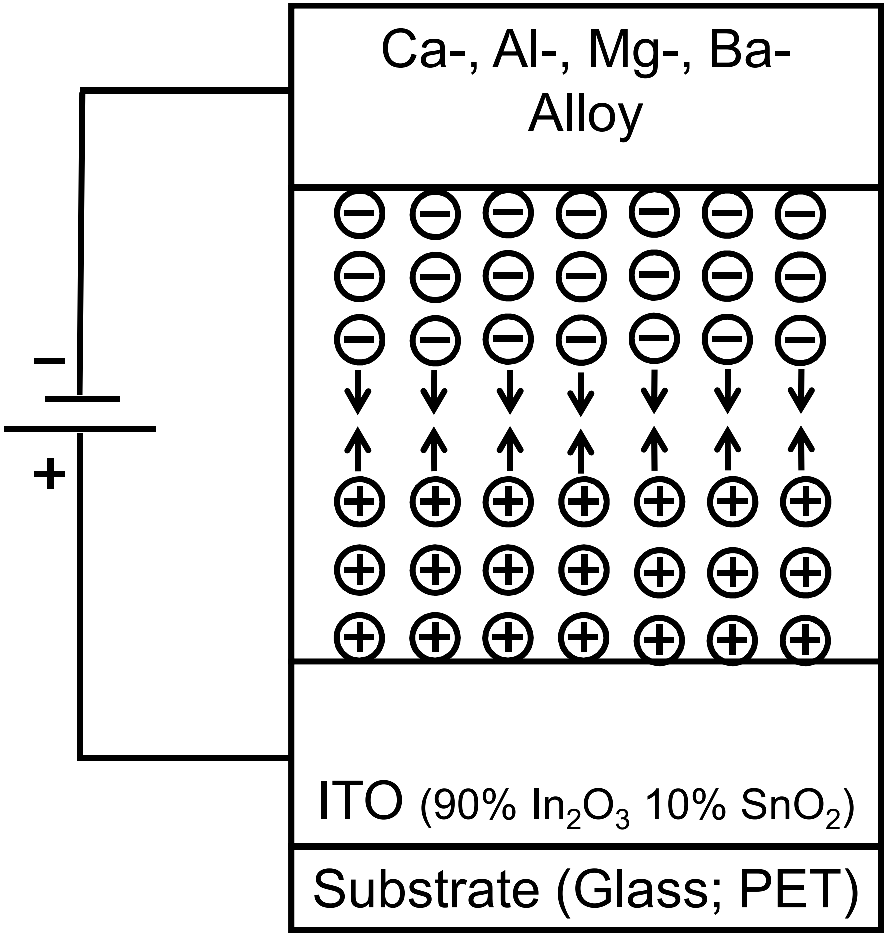
OLED, **O**rganic **L**ight **E**mitting **D**iode, **Single Layer–OLED.**



Progression of the Electron-Hole Migration.

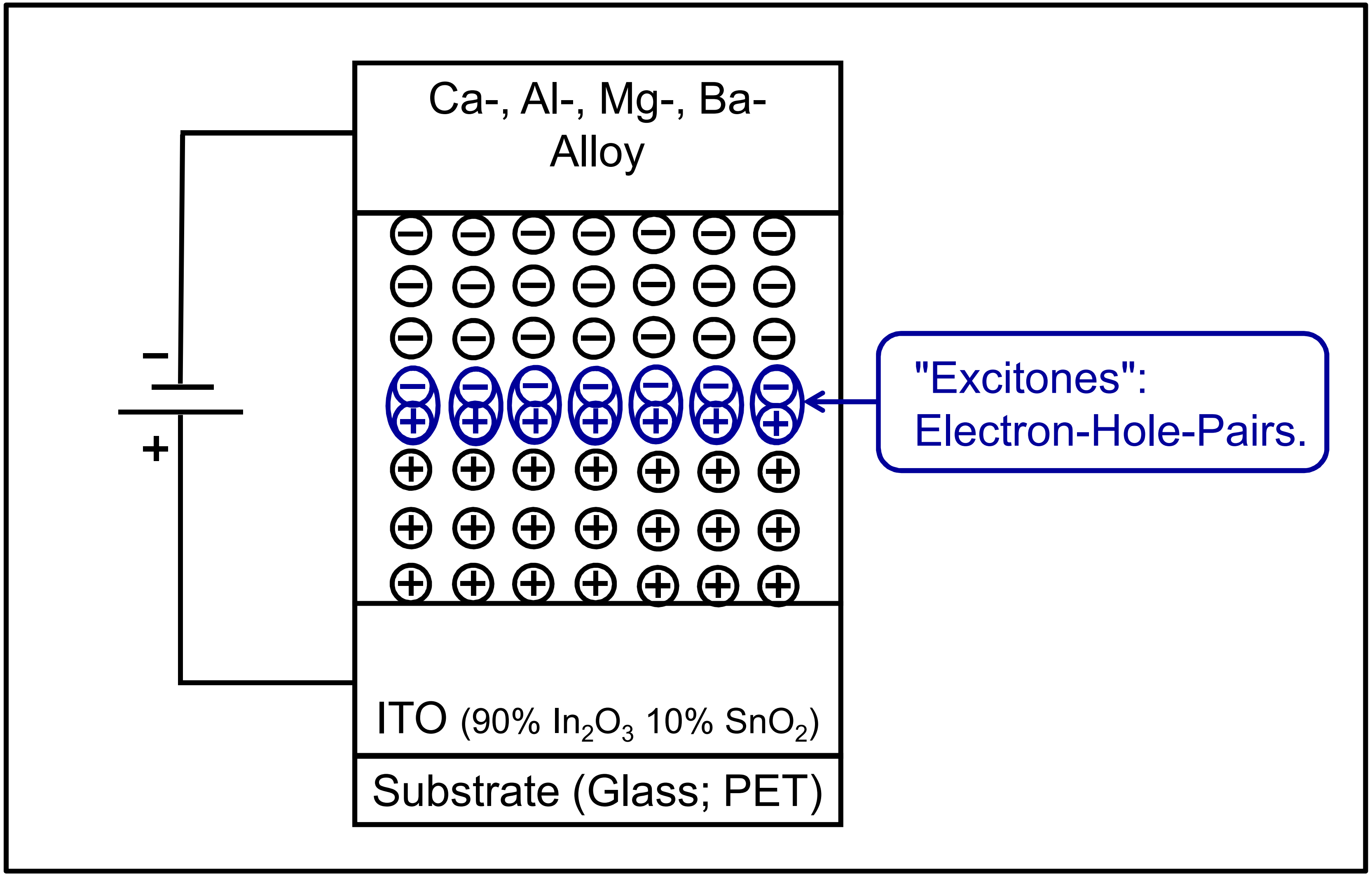
N-Heterocyclic Compounds for OLEDs

OLED, **O**rganic **L**ight **E**mitting **D**iode, **Single Layer–OLED.**



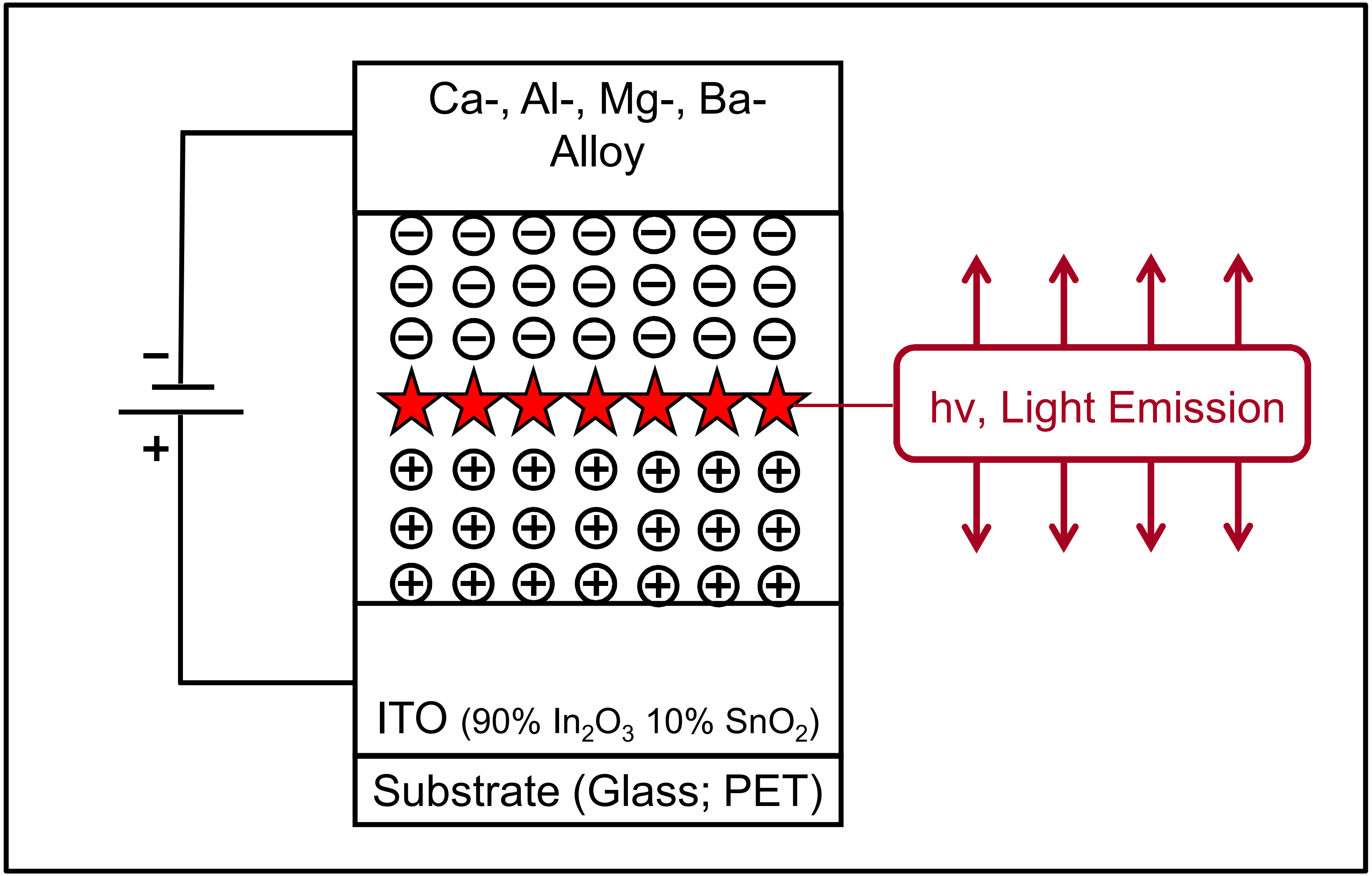
Progression of the Electron-Hole Migration.

OLED, **O**rganic **L**ight **E**mitting **D**iode, **Single Layer–OLED.**



N-Heterocyclic Compounds for OLEDs

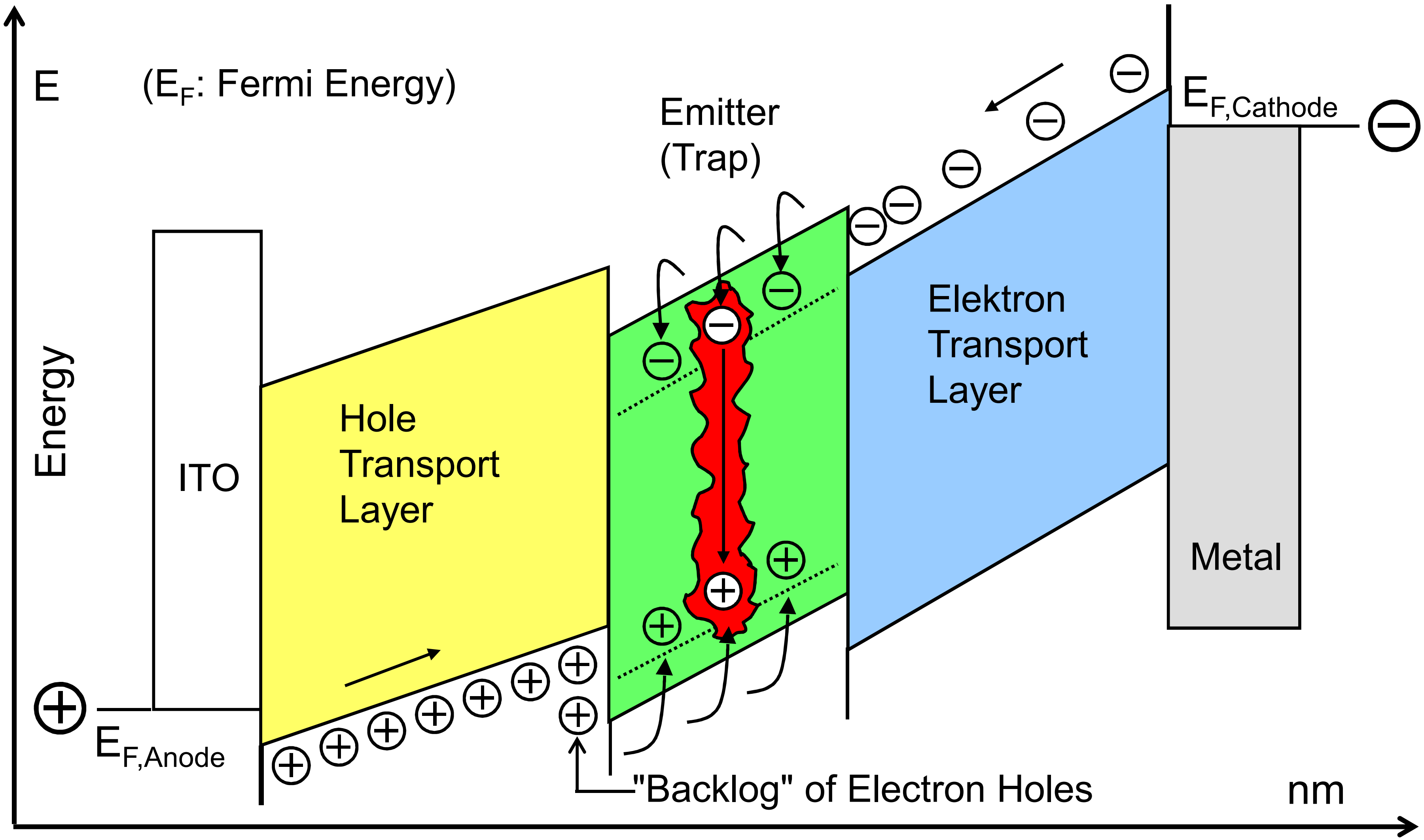
OLED, **O**rganic **L**ight **E**mitting **D**iode, **Single Layer–OLED.**



Rainer Buerstinghaus

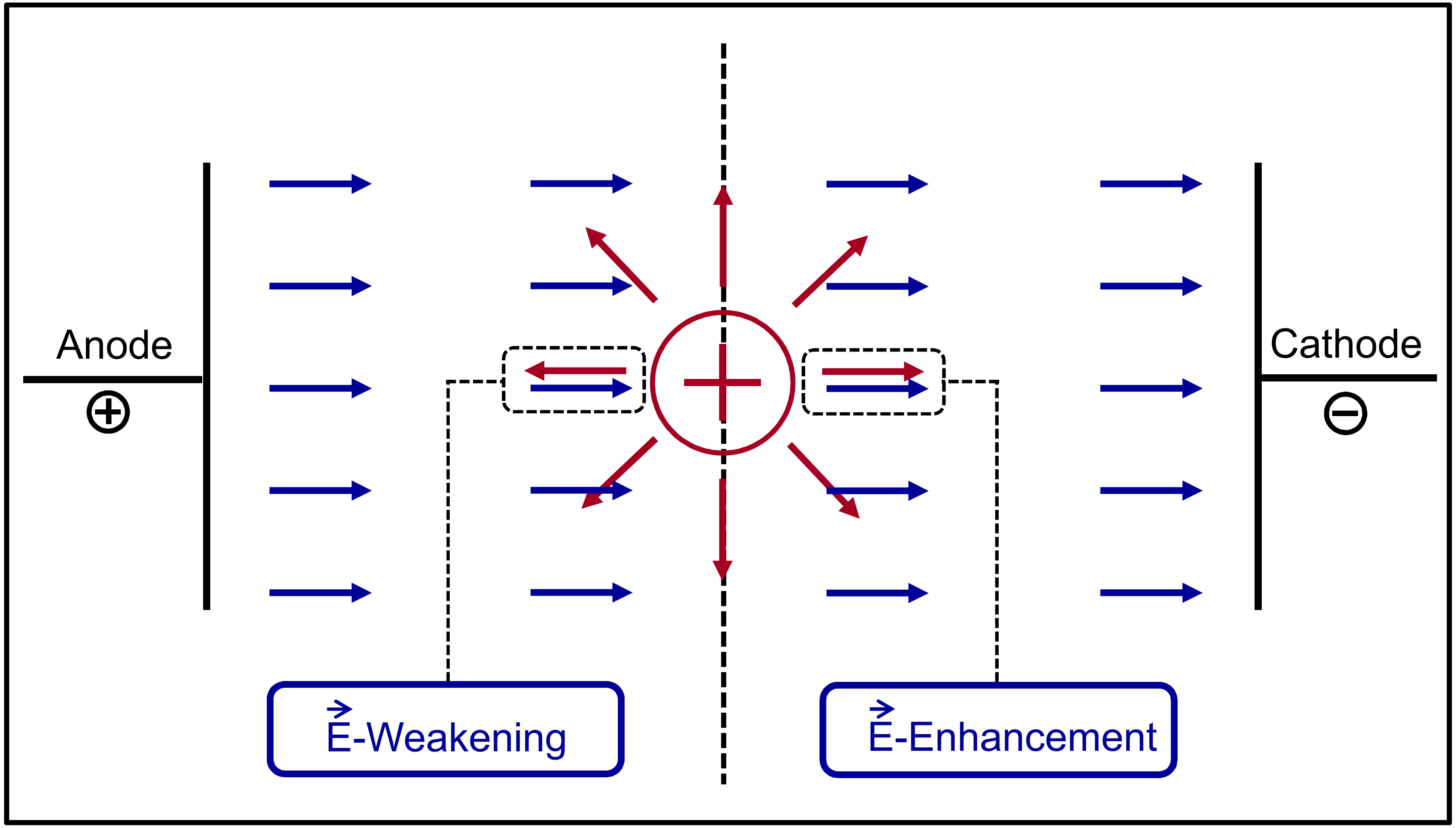
N-Heterocyclic Compounds for OLEDs

Structure of a Light-Emitting Diode with Several Layers.
Energy Levels under Operating Conditions.



Rainer Buerstinghaus

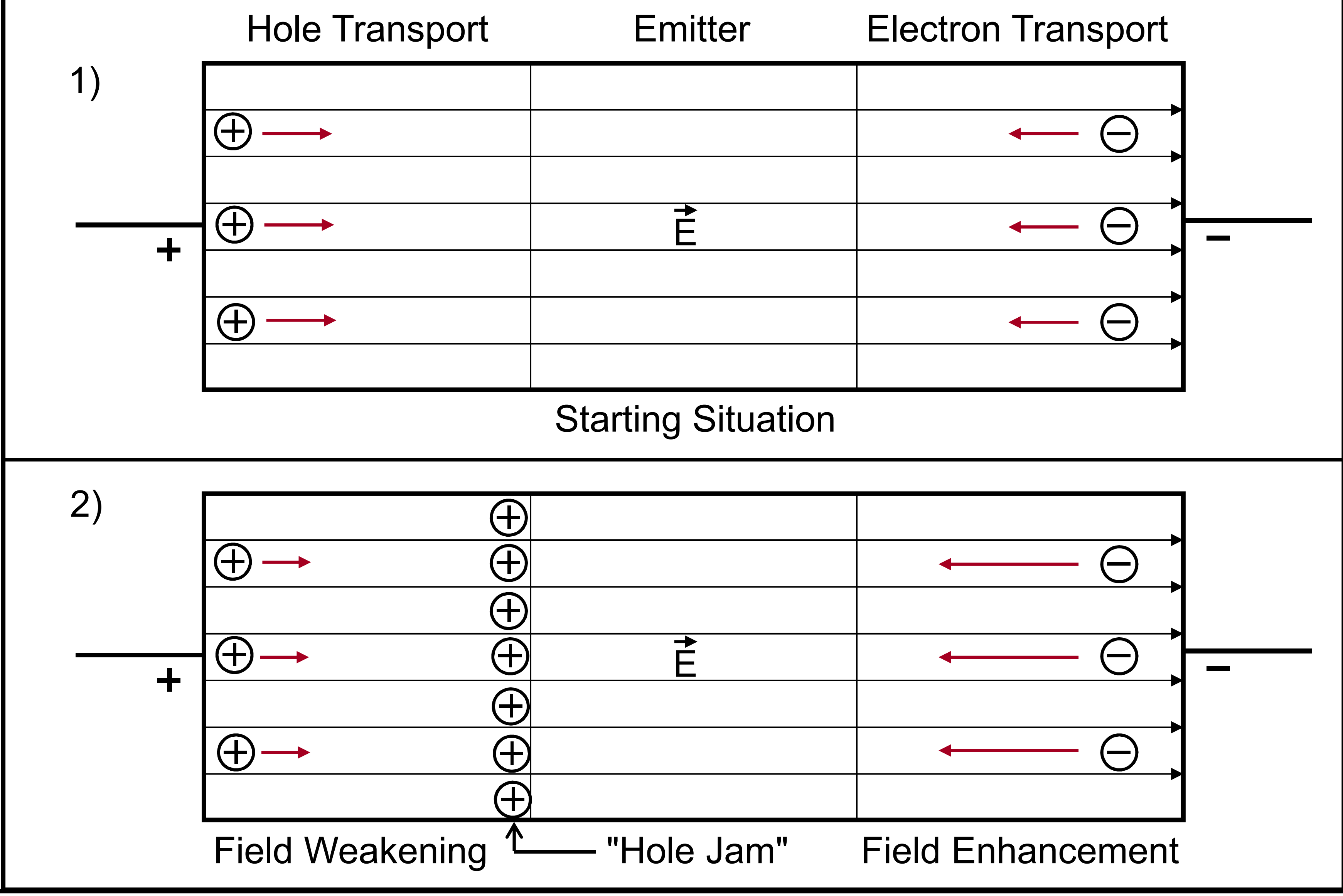
Vectors of the Electric Field $\vec{E}$:
Situation at the Electron Hole (+) Near the Anode, "Hole Jam".



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

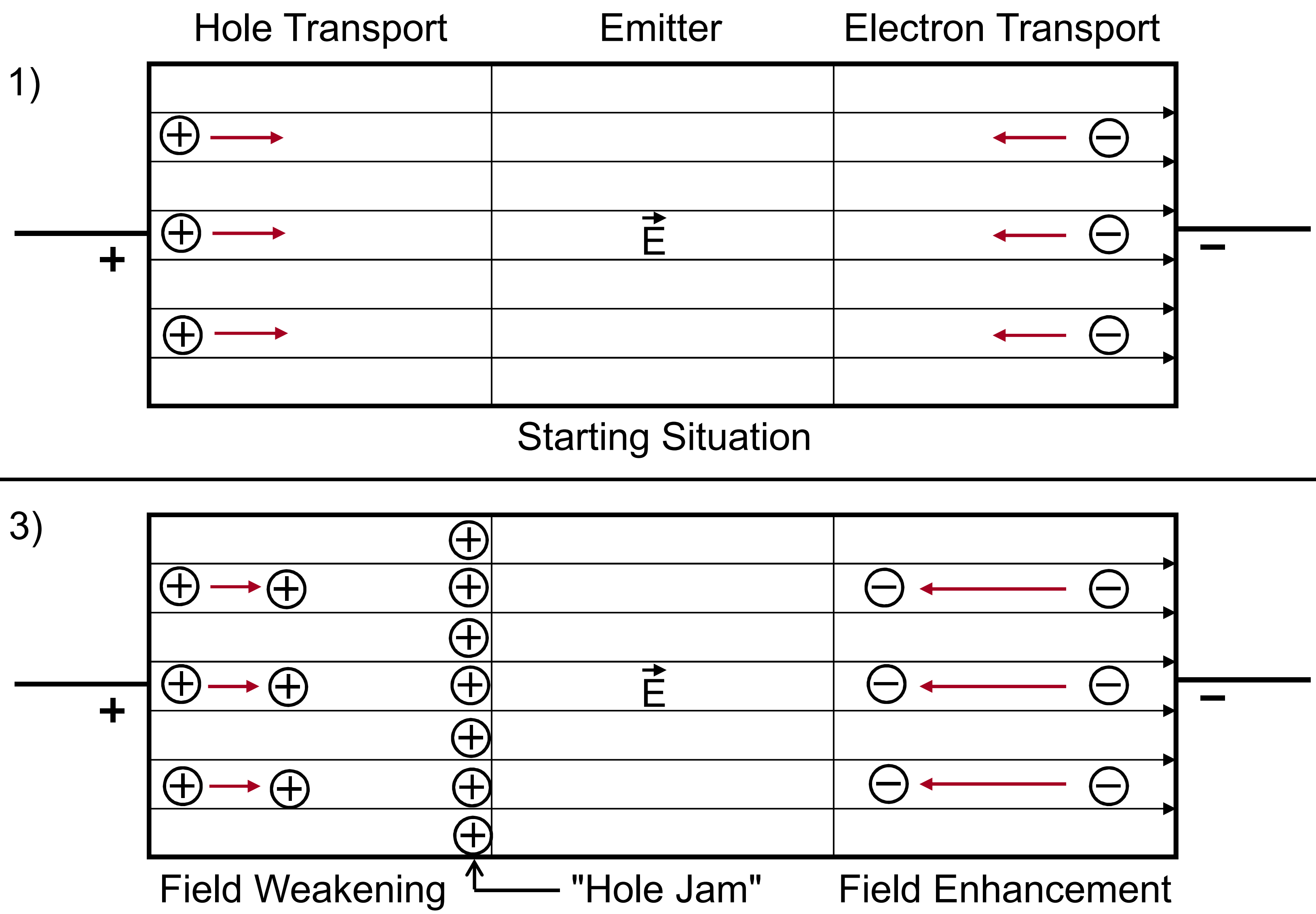
Positive Space Charge Under Operating Conditions.



Rainer Buerstinghaus

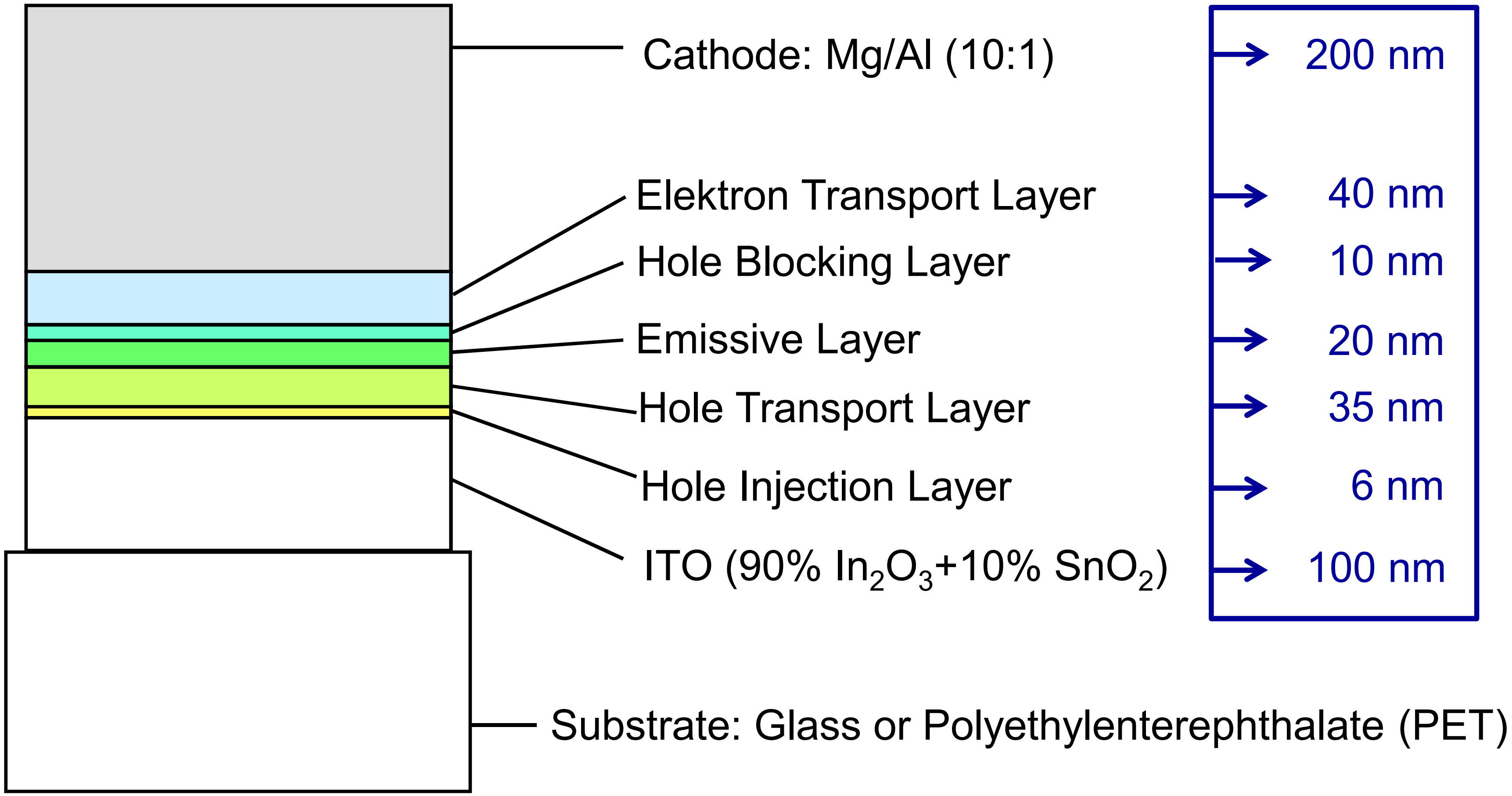
N-Heterocyclic Compounds for OLEDs

Positive Space Charge Under Operating Conditions.

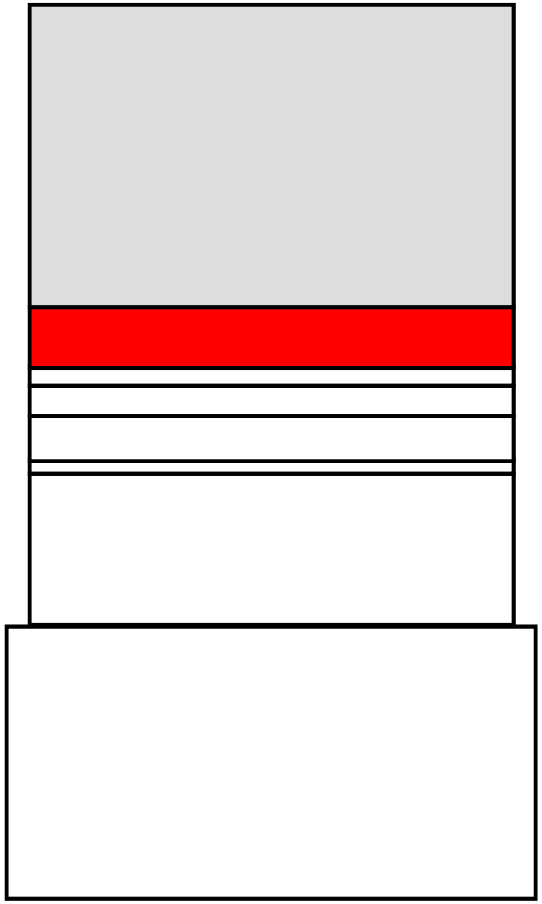


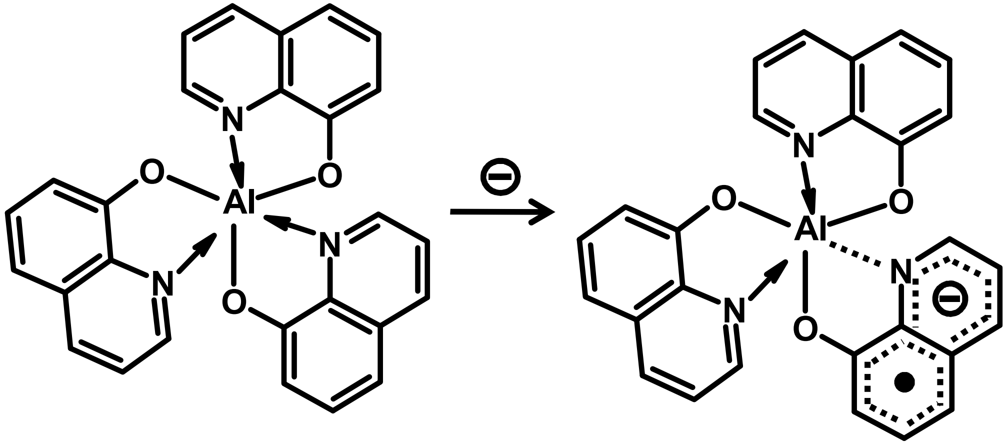
Rainer Buerstinghaus

Multi-Layer Structure of a Phosphorescence OLED.



(Metal)Organic Electron Transport Layer; Structure Example.

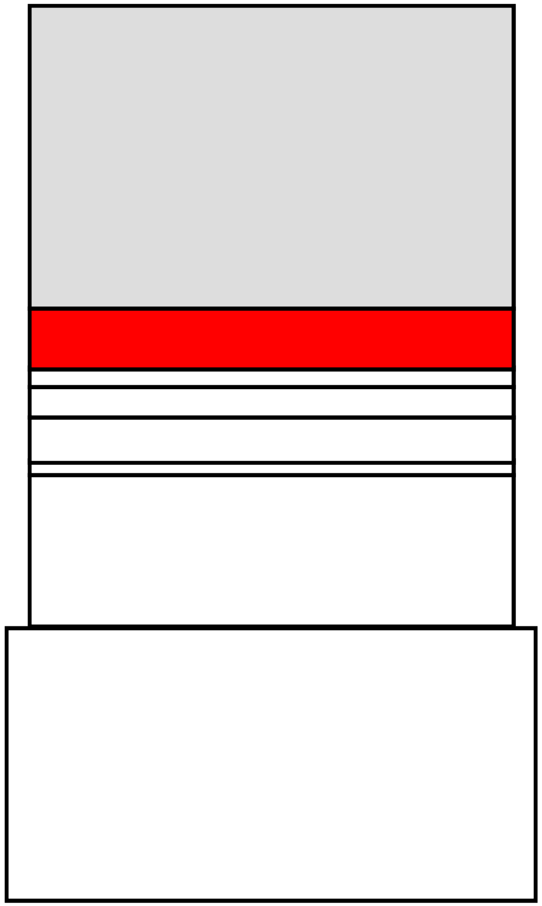


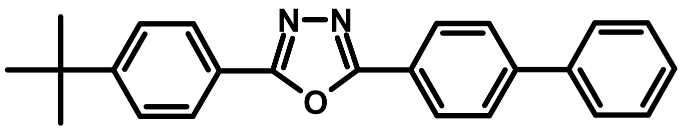


"Electron transporter" aluminum oxinate: Electron uptake to the radical anion with a delocalized electrical charge.

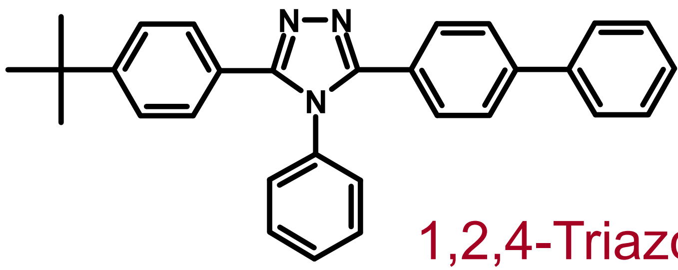
N-Heterocyclic Compounds for OLEDs

(Metal)Organic Electron Transport Layer; Structure Examples.

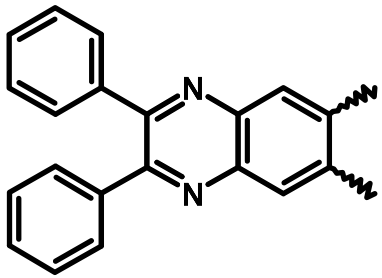




1,3,4-Oxadiazole Type



1,2,4-TriazoleType

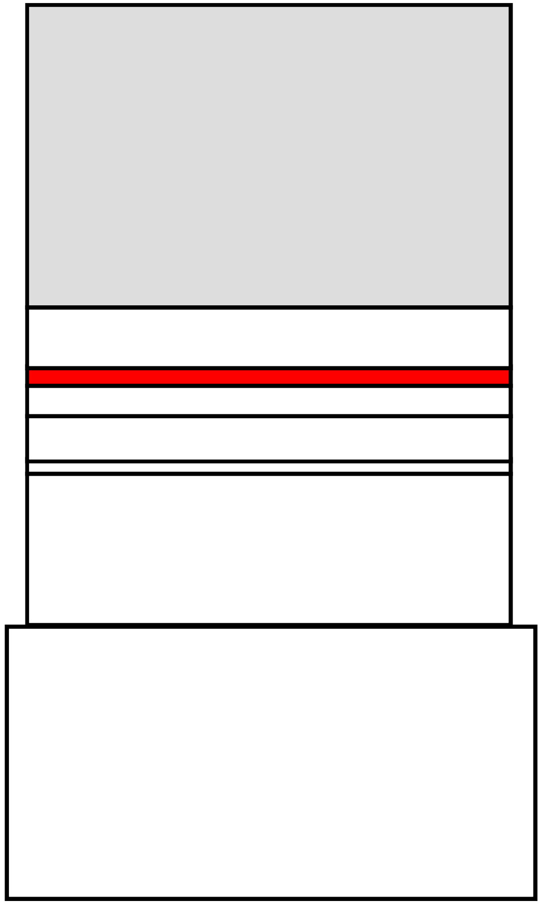


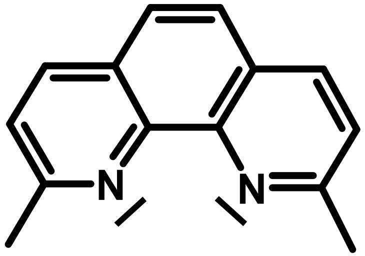
Quinoxaline Type

Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

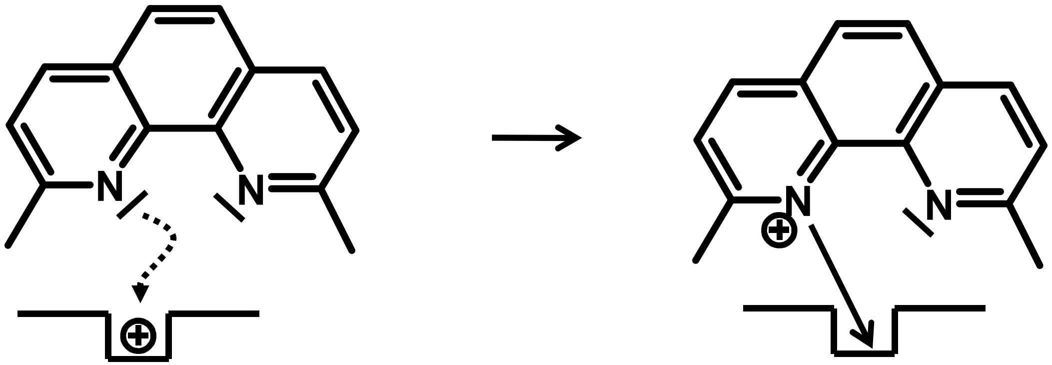
Organic Hole Blocking Layer; Structure Example.





2,9-Dimethyl-1,10-Phenanthroline

Mechanism of Blocking:



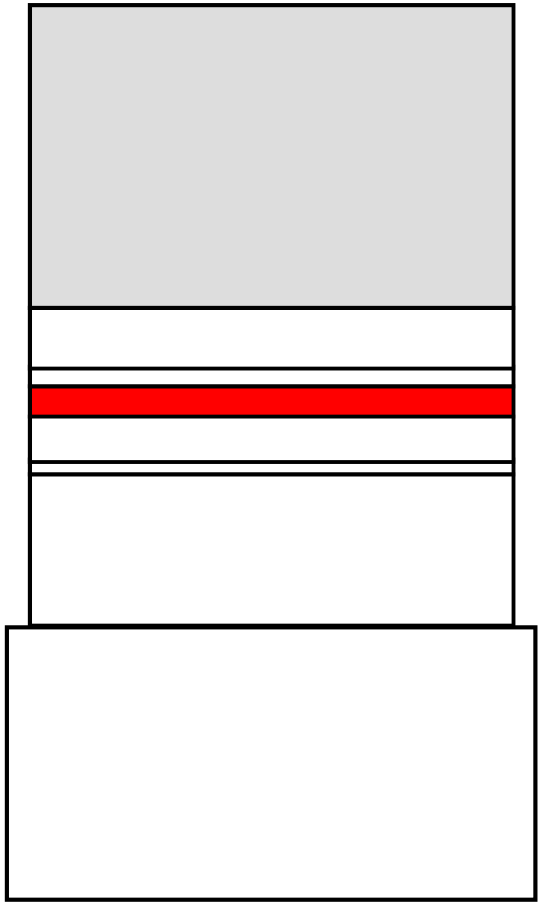
Electron hole:
A non-recombined "defec-tor" from the emitter layer.

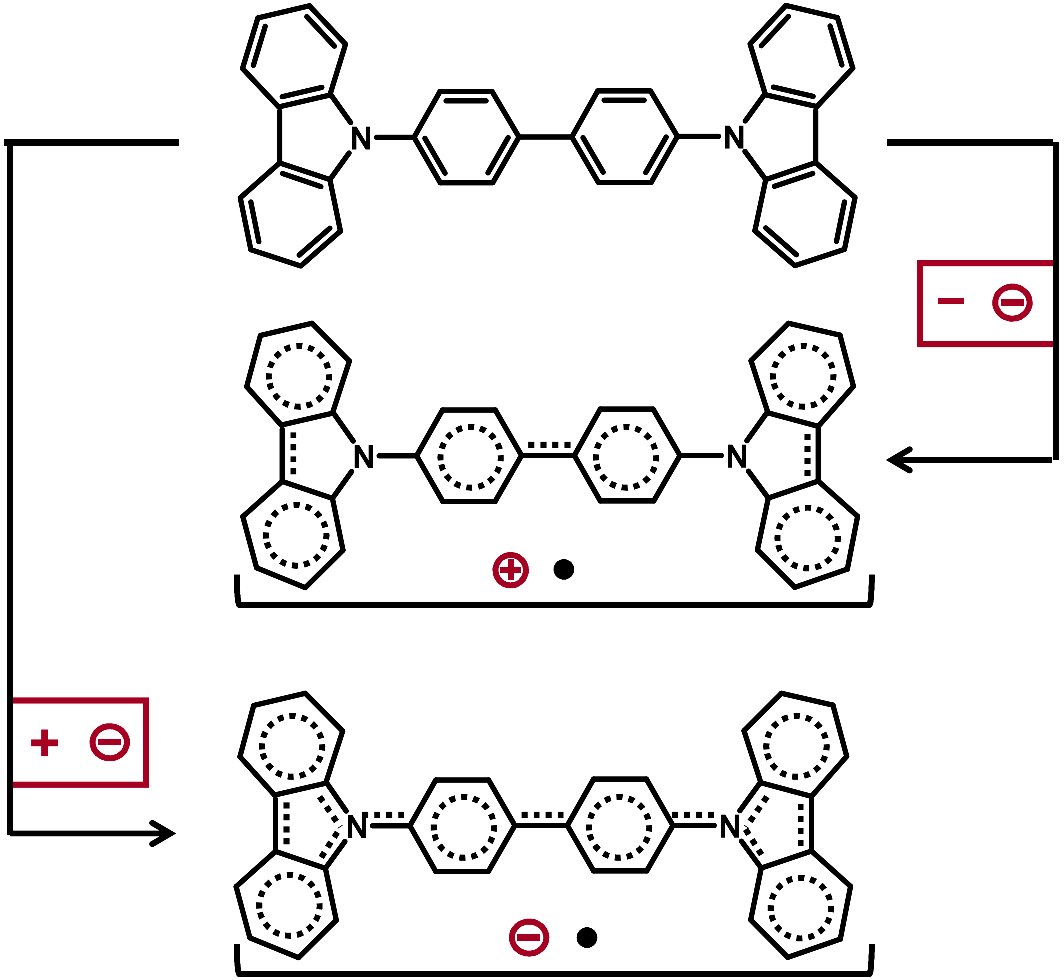
Cationic "energy level trap" :
There is no further intermole-cular, "saltatory" forwarding.

Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

Organic Emissive Layer (Recombination Layer); Structure Example, Electron Uptake, Electron Release.

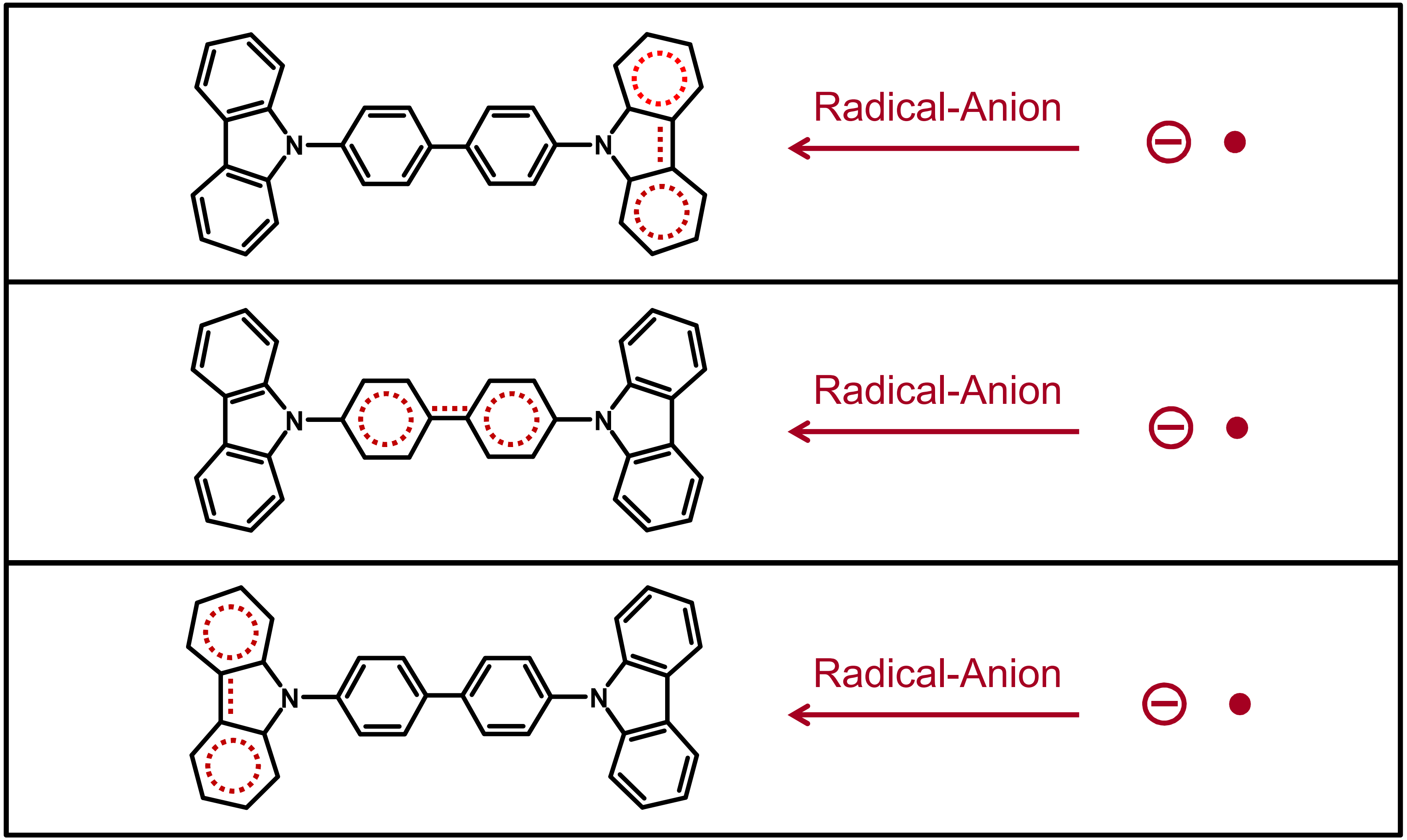




Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

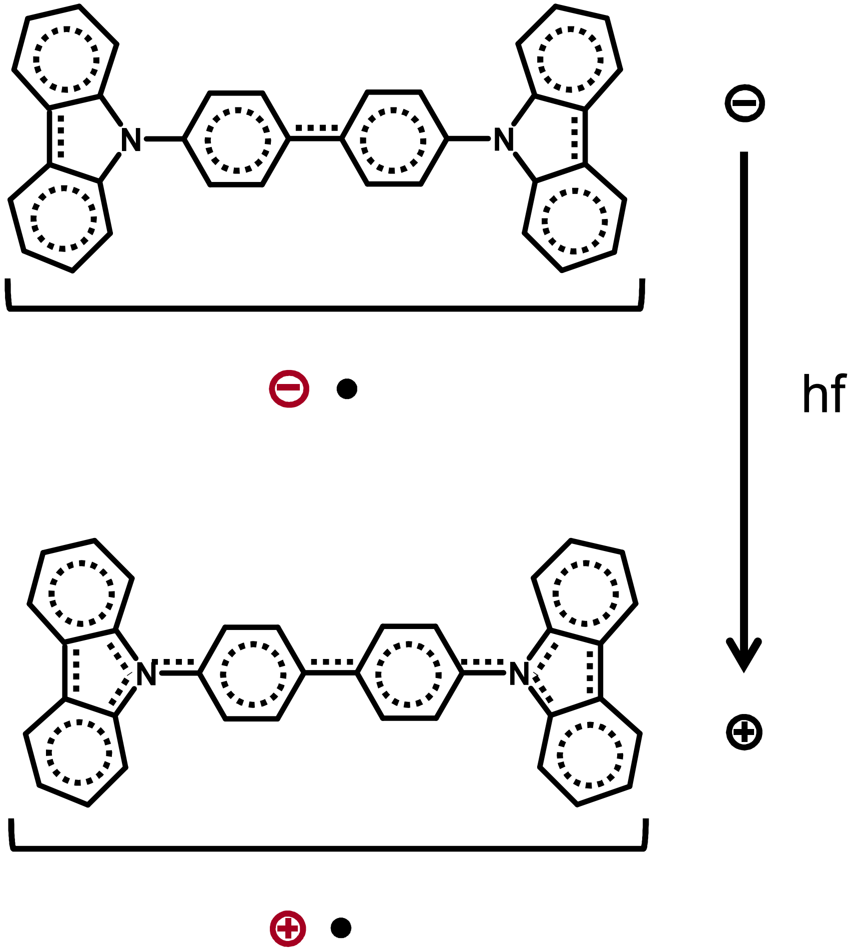
Organic Emissive Layer: Structure Example; Three Zones with the Possibility of Electron Uptake.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

Organic Recombination Layer: Exciton.

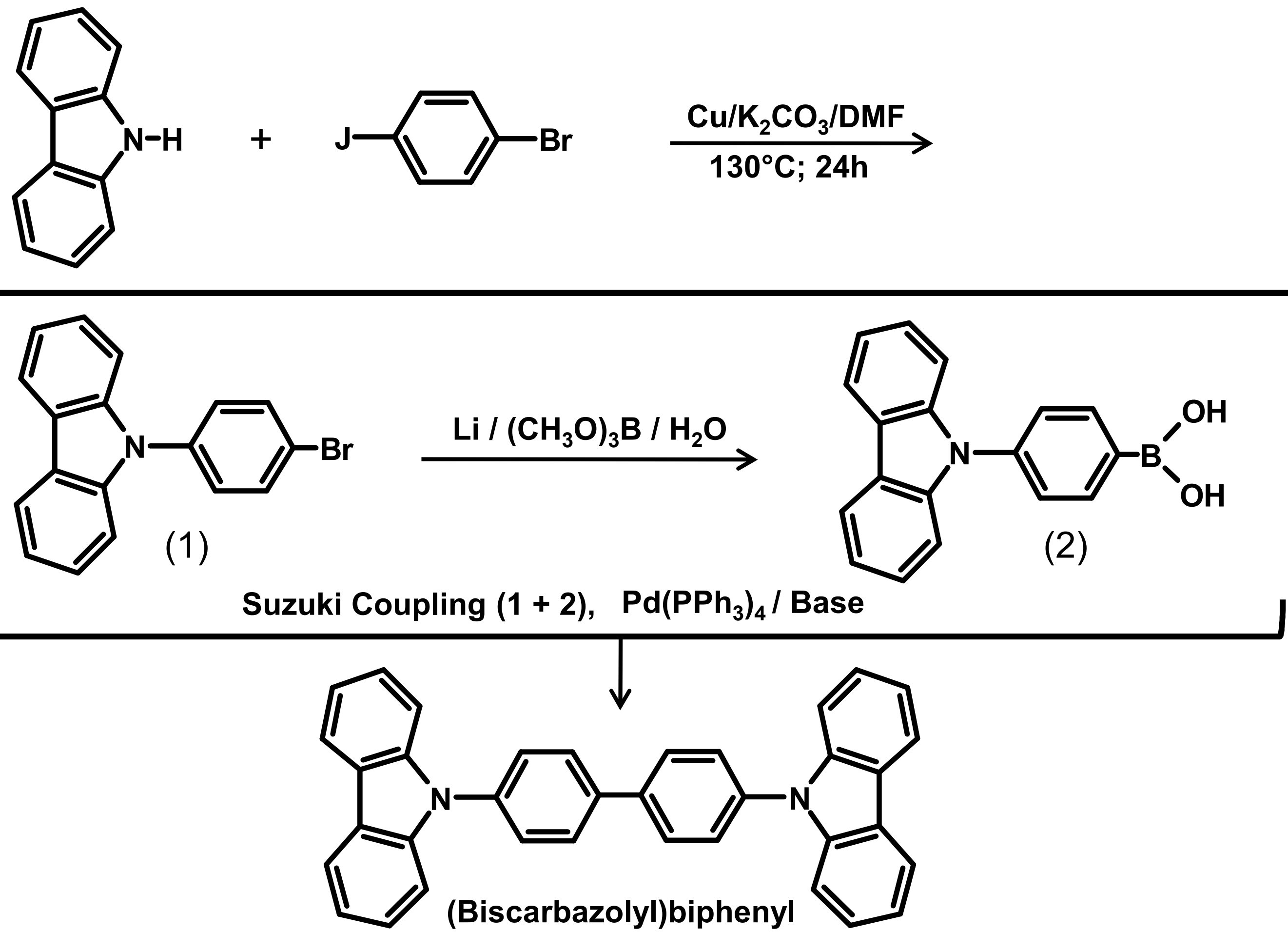


Exciton

Electron-hole pair, which is held together by the (+ / −) Coulomb force. Towards the exterior, it is a neutral quasiparticle with integer spin that moves in the semiconductor crystal as the "transporter" of the excitation energy.

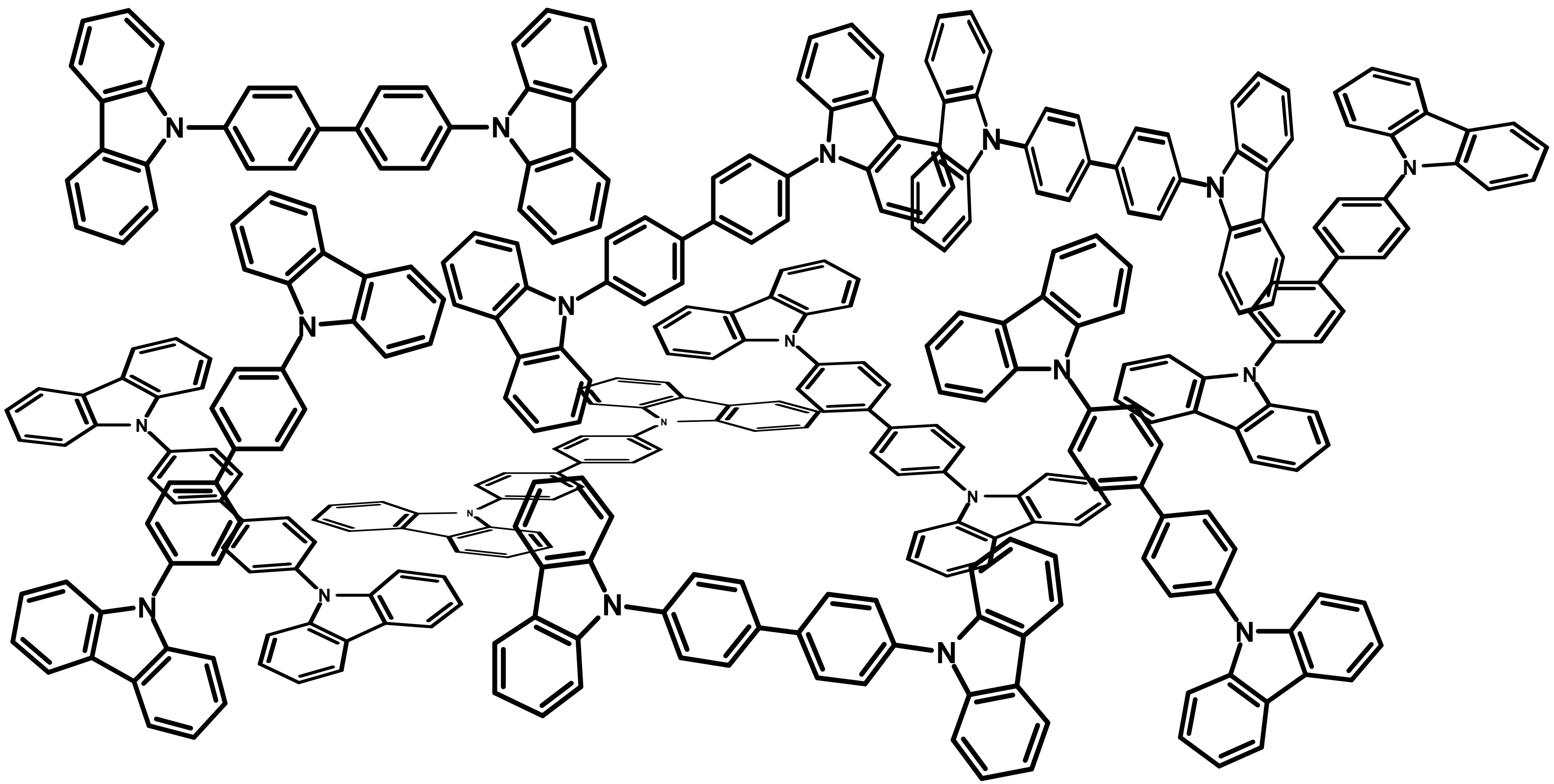
Rainer Buerstinghaus

Recombination Layer, Emissive Layer, Chemistry; Synthesis of the BCBP Using a Suzuki Coupling.



N-Heterocyclic Compounds for OLEDs

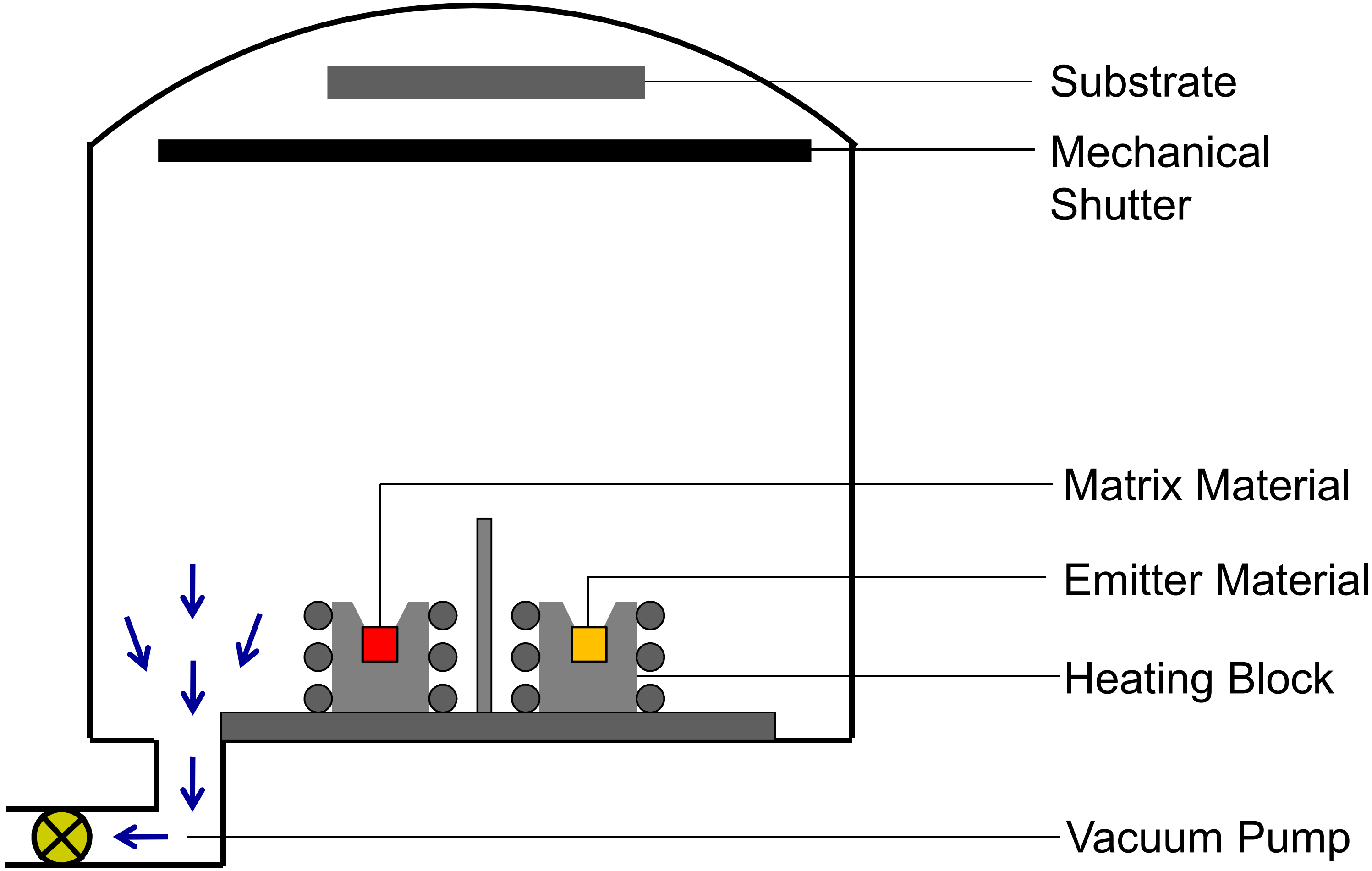
OLED, Conjugated Aromatics (Single Molecules);
Application of the Molecules by "Thermal Vacuum Evaporation":
Glass-Like, Non-Crystalline, Molecular Accumulation.



Rainer Buerstinghaus

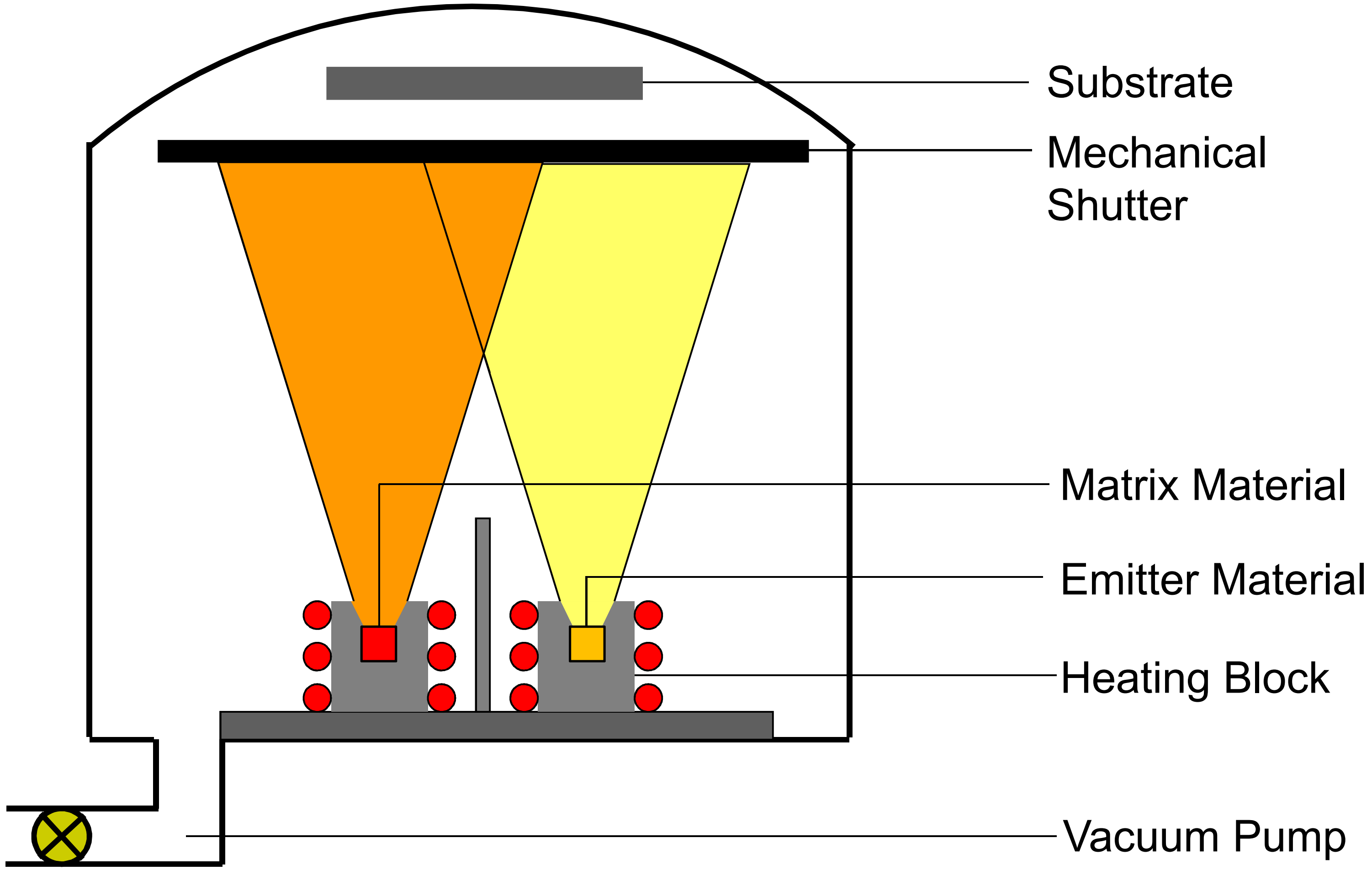
N-Heterocyclic Compounds for OLEDs

Thermal Vacuum Evaporation, Experimental Set-up; Heating Switched Off, Closed Mechanical Shutter.



N-Heterocyclic Compounds for OLEDs

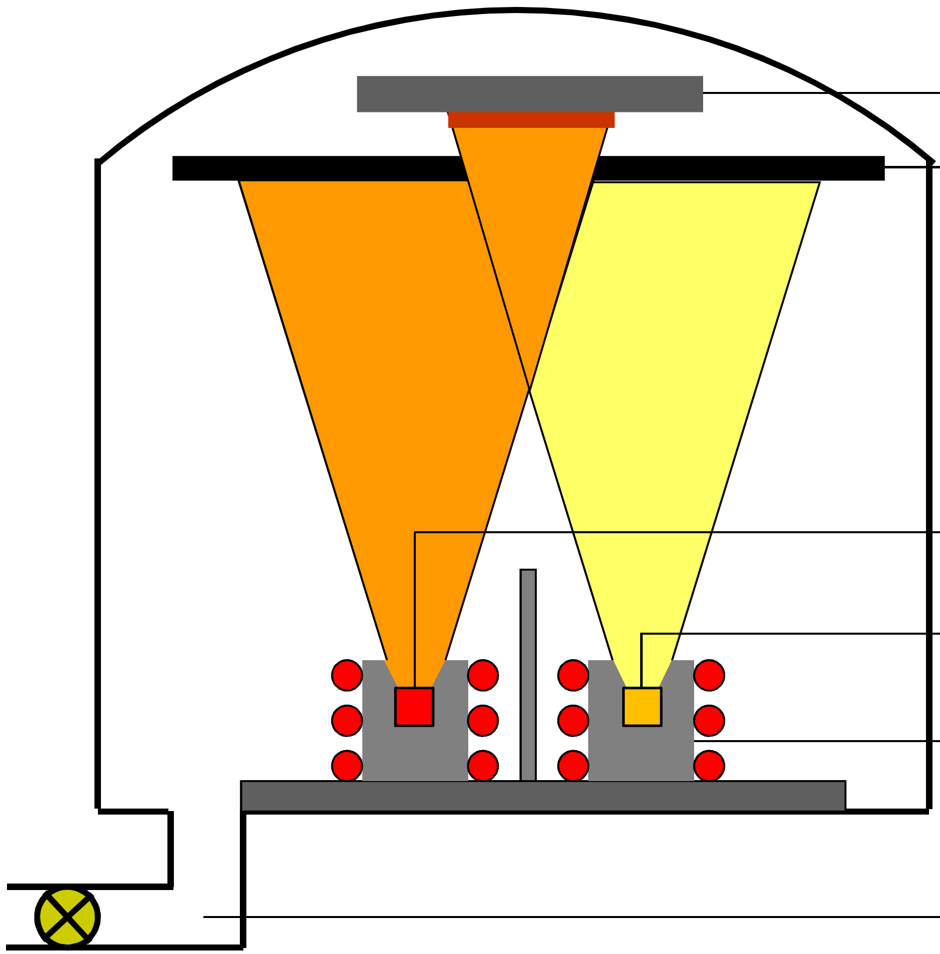
Thermal Vacuum Evaporation, Experimental Set-up; Heating Switched On, Closed Mechanical Shutter.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

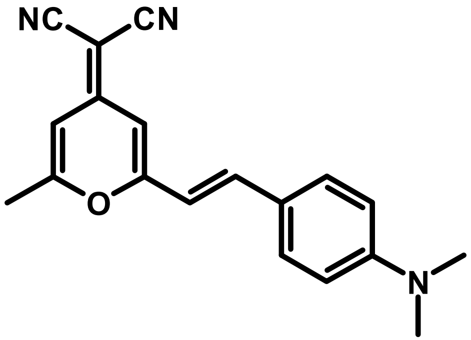
Thermal Vacuum Evaporation, Experimental Set-up; Heating Switched On, Opened Mechanical Shutter.



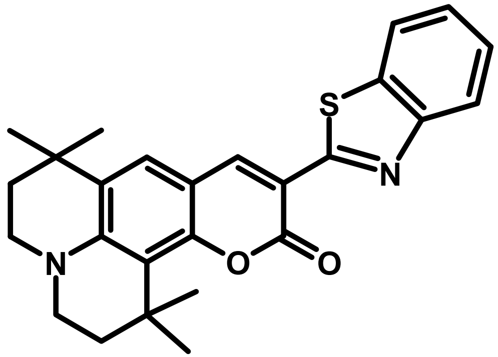
Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

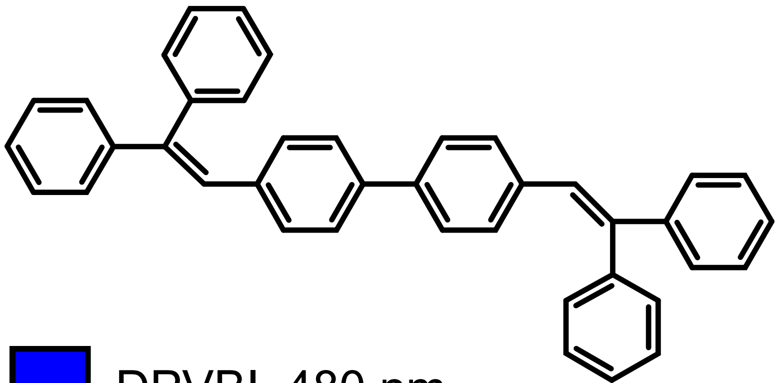
Electroluminescent Dyes, Structure Examples.



DCM, 627 nm



Cumarin C545T, 550 nm

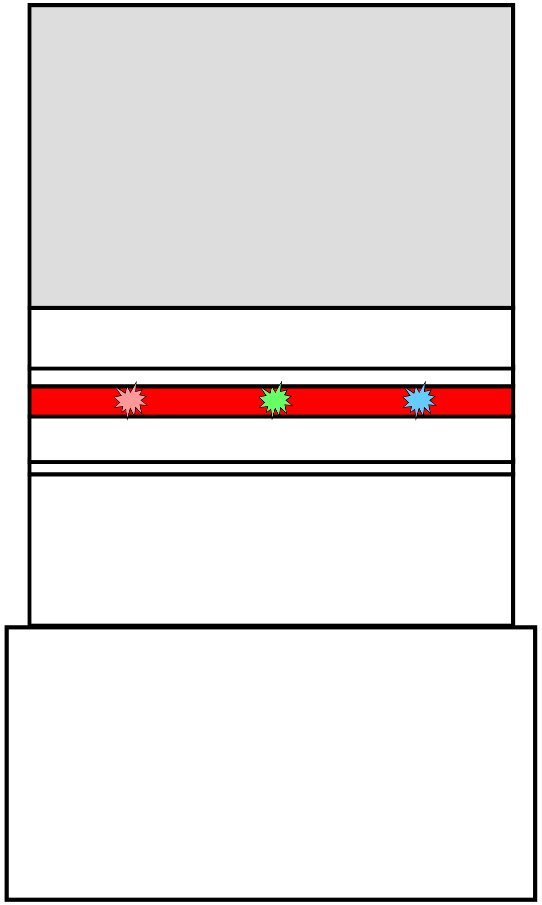


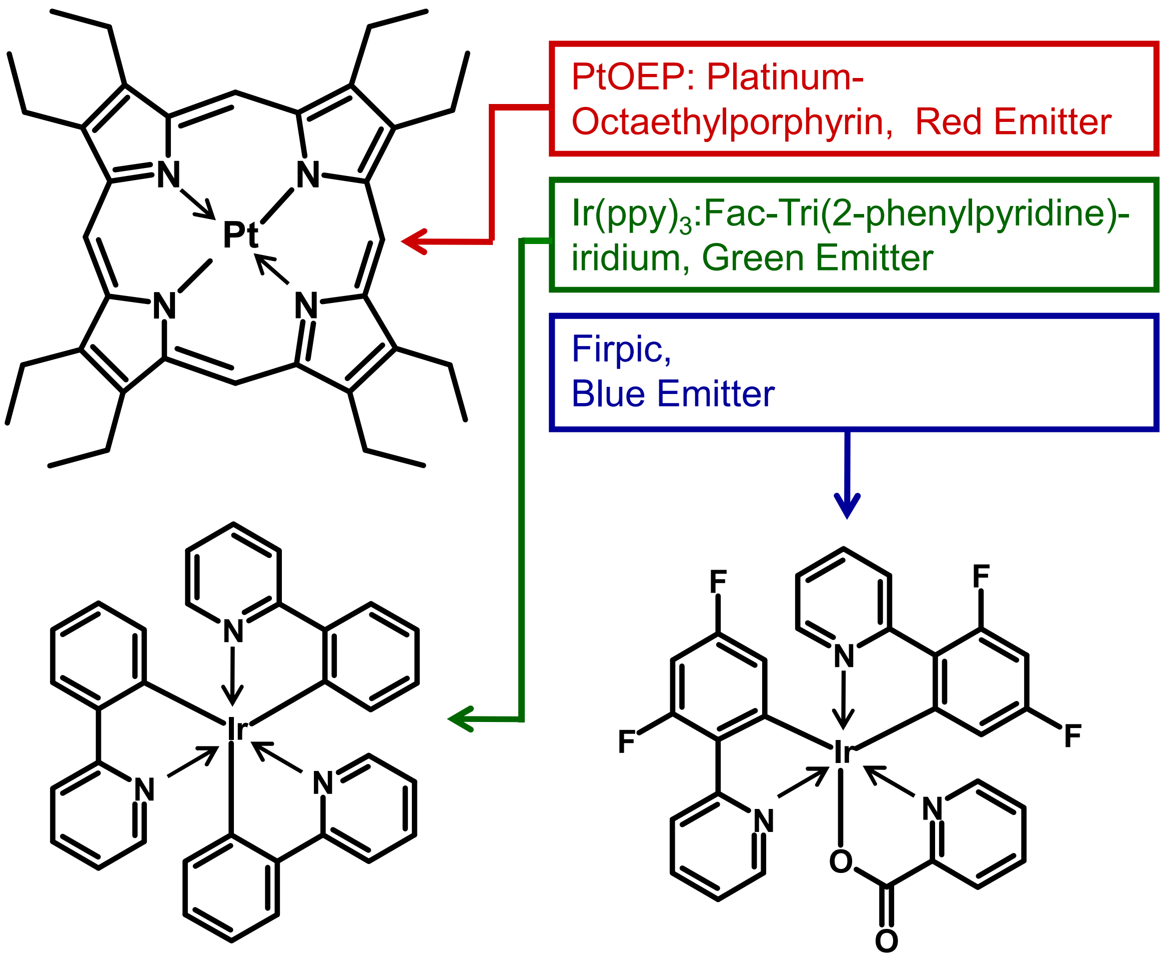
DPVBI, 480 nm

Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

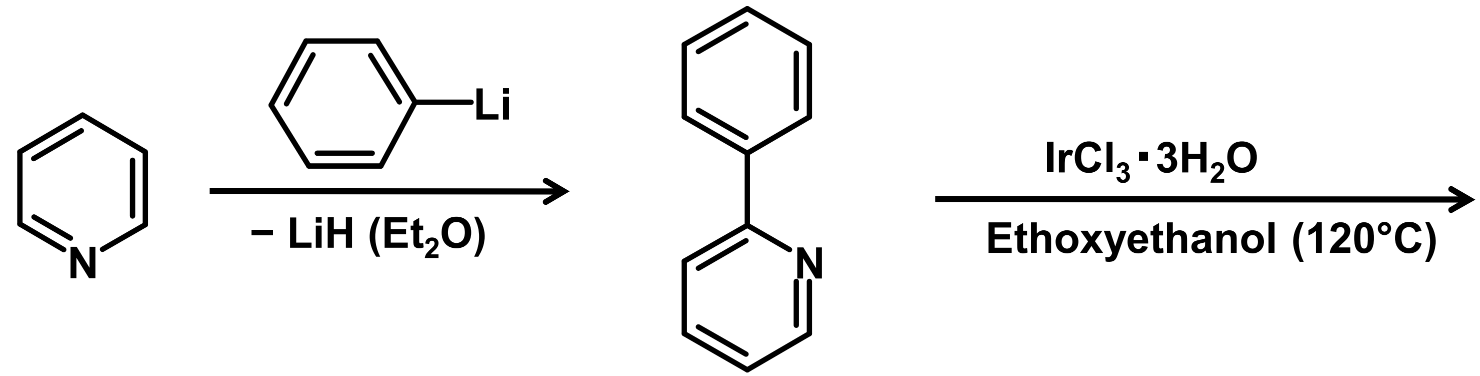
Recombination Layer, Emissive Layer: Triplet Emitters with Platinum Metals as "Inductors", Structure Examples.

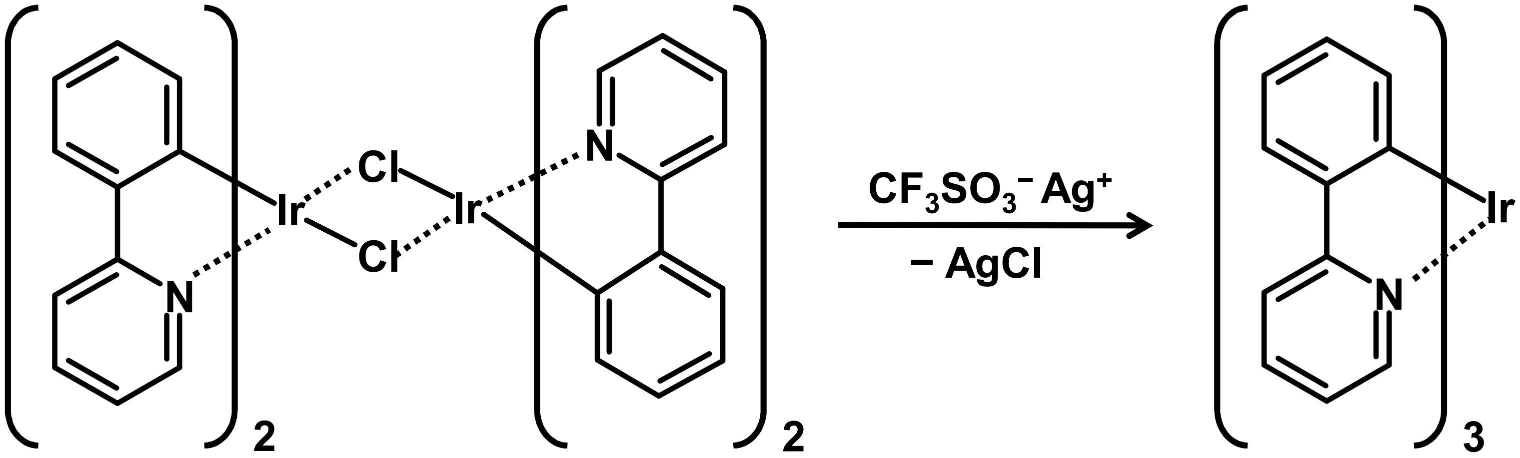




Rainer Buerstinghaus

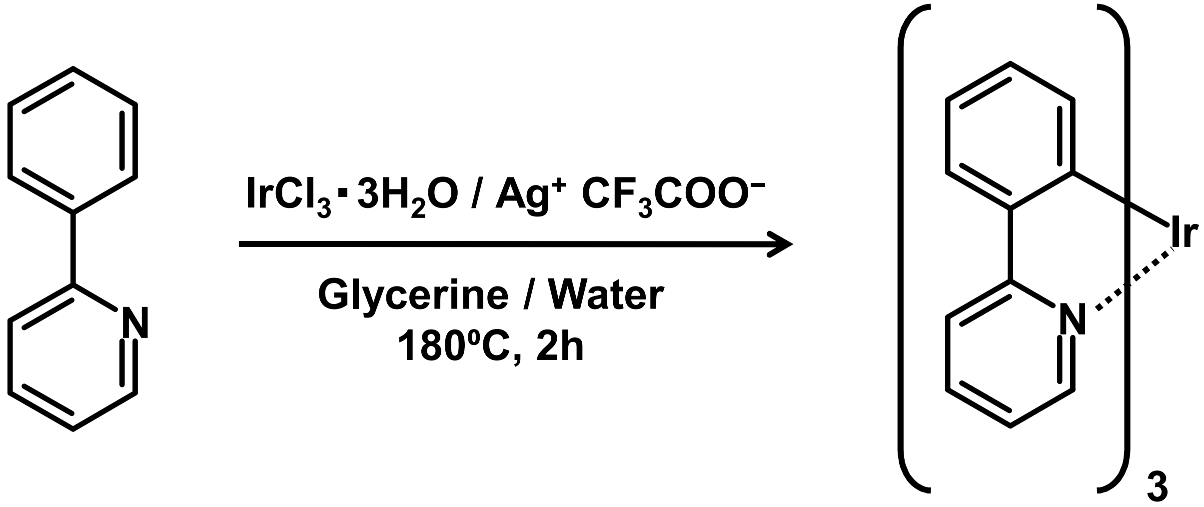
Synthesis of Ir(ppy)$_3$ from Pyridine and Phenyllithium.





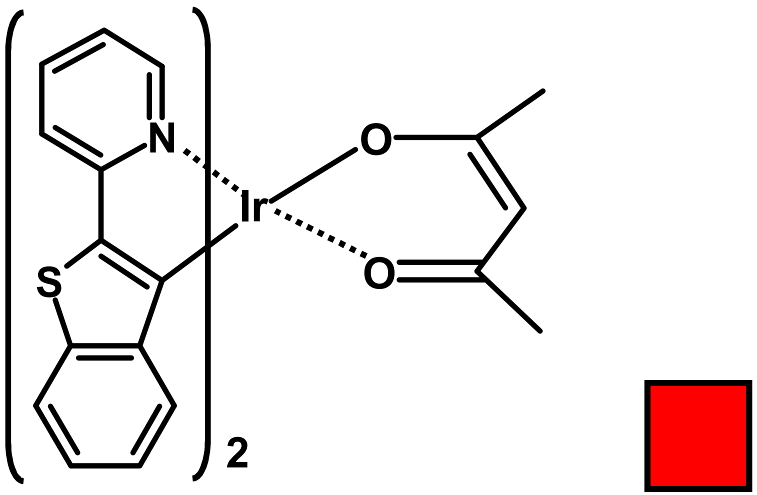
Rainer Buerstinghaus

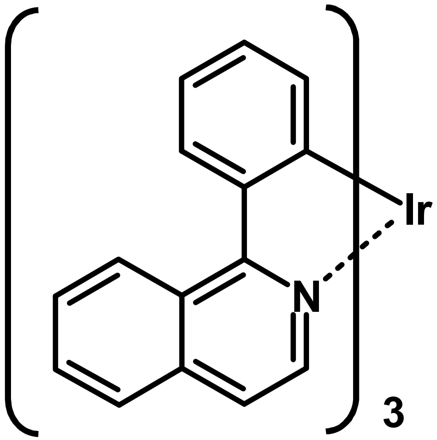
One-Step Synthesis of $Ir(ppy)_3$.

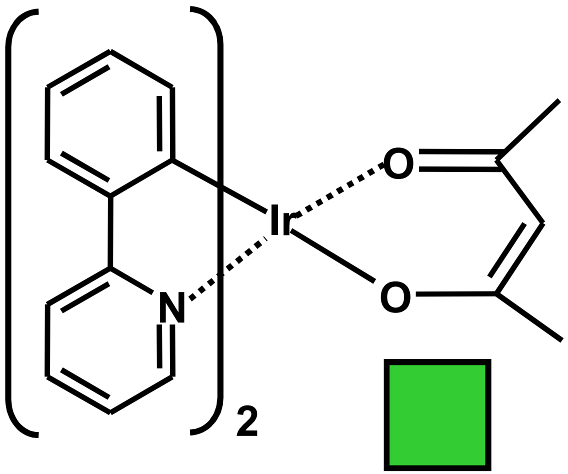


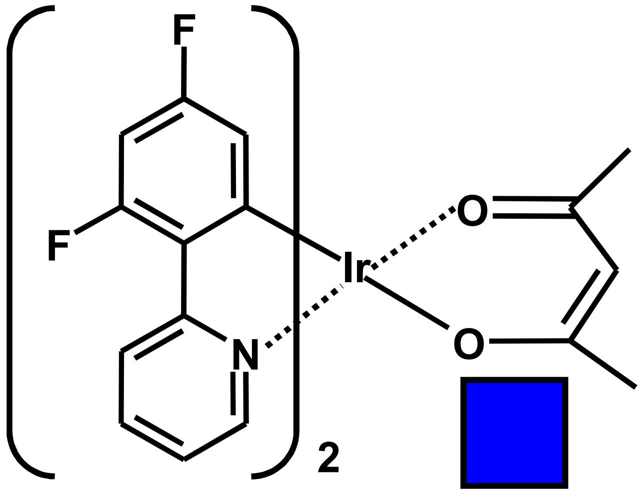
N-Heterocyclic Compounds for OLEDs

More Triplet Emitters, Structure Examples.



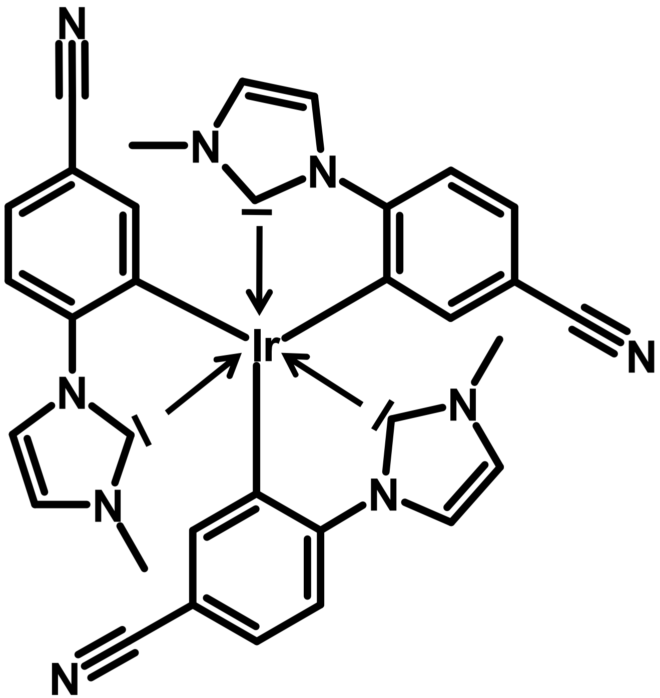




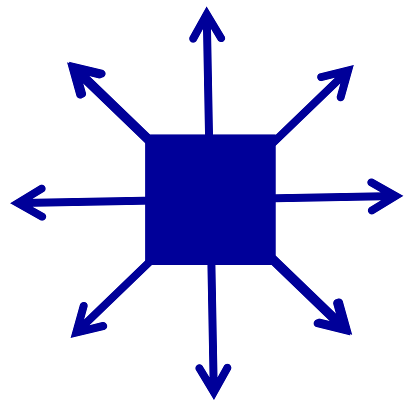


Rainer Buerstinghaus

Another Triplet Emitter, Structure Example.



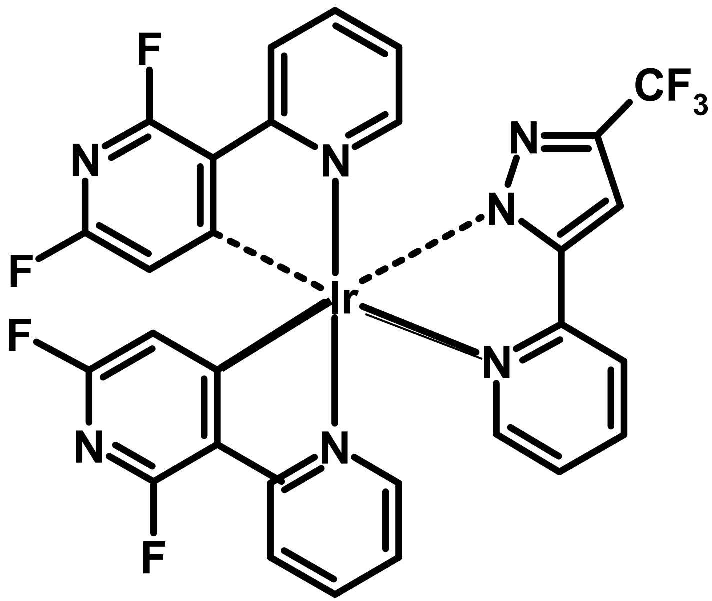
Ir-NHC:
Ir-N-Heterocyclic Carbene



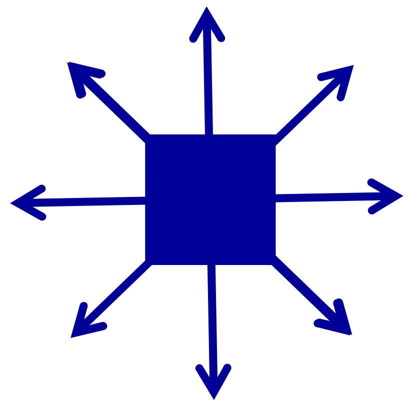
Ir (cn-ptnic) $_3$:
Carbene Triplet Emitter: Intensive **Blue Light** Emission.

N-Heterocyclic Compounds for OLEDs

Another Triplet Emitter, Structure Example.



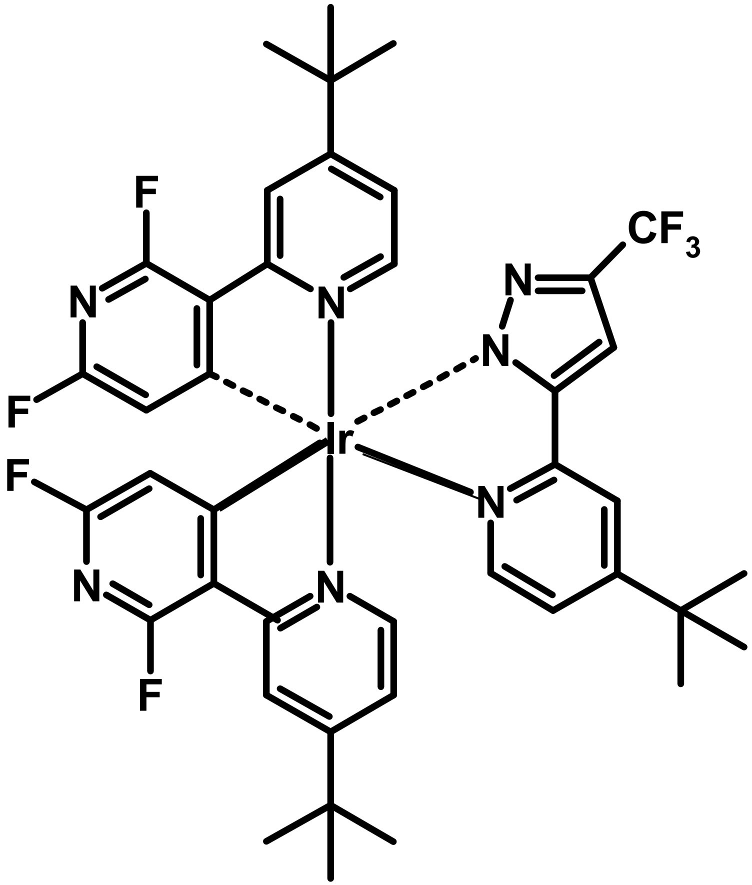
Ir-(dfpypy)$_2$(fppz)
Ir-Heteroleptic Complex



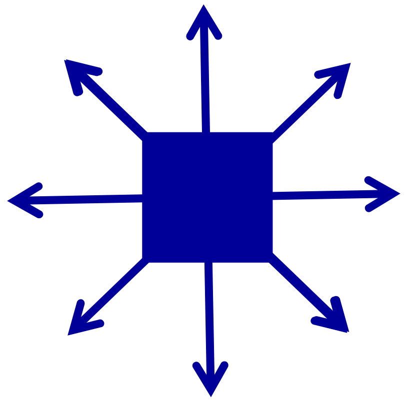
Ir-(dfpypy)$_2$(fppz):
Ir (III) Complex with Intensive **Blue Light** Emission.

N-Heterocyclic Compounds for OLEDs

Another Triplet Emitter, Structure Example.

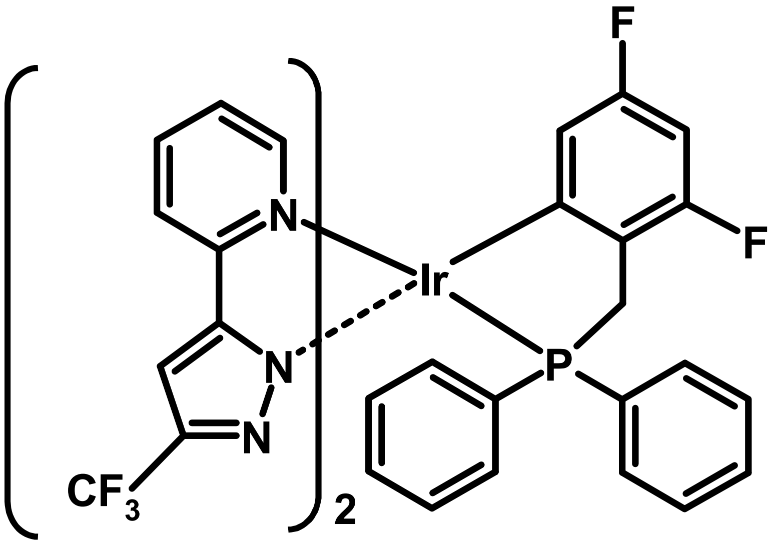


Ir-(dfpybpy)$_2$(fpbpz)
Ir-Heteroleptic Complex

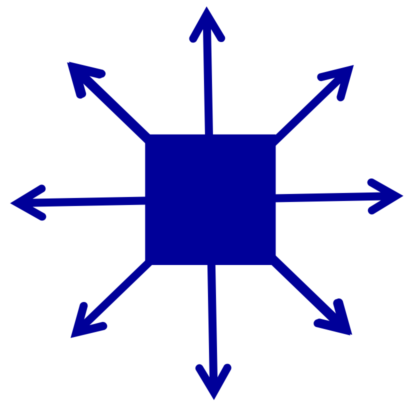


Ir-(dfpybpy)$_2$(fpbpz):
Ir (III) Complex with Intensive **Blue Light** Emission.

Another Triplet Emitter, Structure Example.

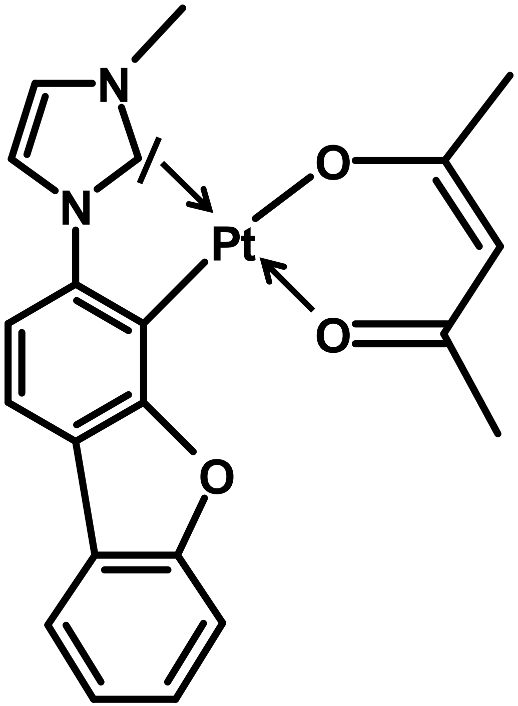


Ir-Phosphane-Complex

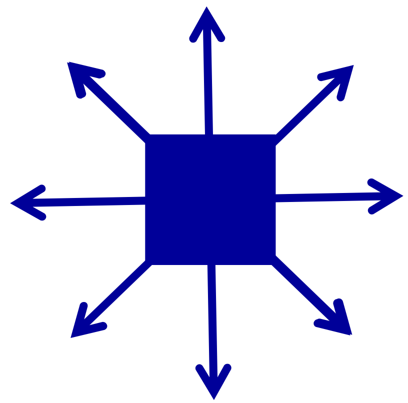


Ir (III) Complex with Intensive **Blue Light** Emission.
(Yang, Xu, Zhou, 2015)

Another Triplet Emitter, Structure Example.



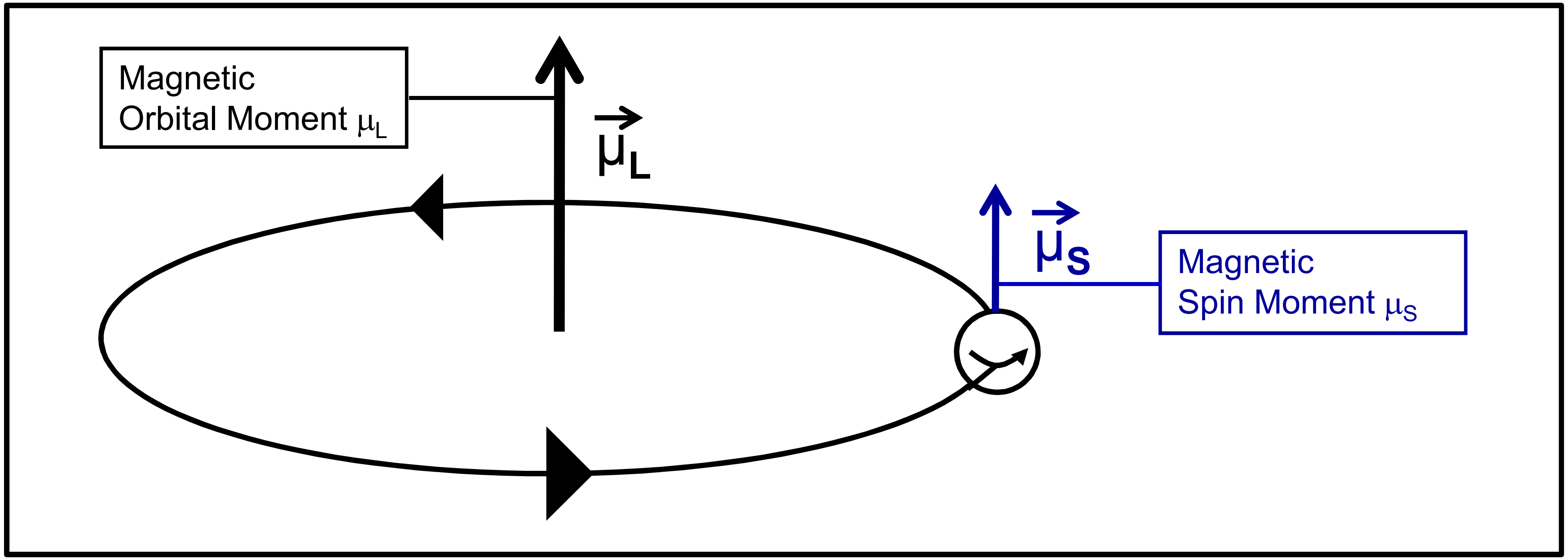
Pt-NHC:
Pt-N-Heterocyclic Carbene



Carbene Triplet Emitter with intensive
Blue Light Emission (BASF SE, 2010)

Triplet Emitter, Spin-Orbit Interaction.

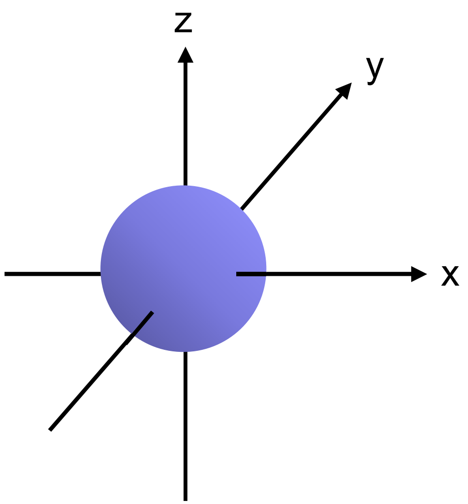
Singlet state ⟶ Triplet state (Intersystem Crossing, ISC):
Only possible with a large spin-orbit interaction in the presence of "heavy" atoms.
The spin-orbit interaction is magnetic in nature.



Spin Angular Momentum (S) + Orbital Angular Momentum (L) =
Total Angular Momentum (J) ⟶ S + L = J.
The interaction between the therewith associated μ_S and μ_L is ~ Z^4 (!);
(Z = Atomic Number = Proton Number).

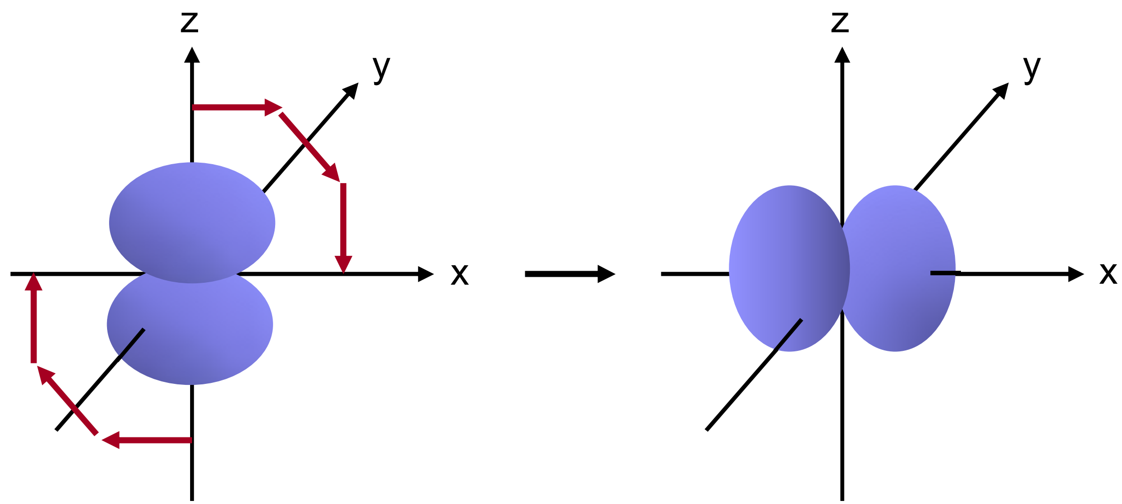
Triplet Emitter, Spin-Orbit Interaction.

In order for an atom-bound electron to have an orbital angular momentum, it must be possible to convert the occupied orbital by rotation into a completely equivalent, degenerate orbital:



s Orbital

1s (n=1, L=0)
2s (n=2, L=0)



p Orbital

2p (n=2, L=1)
3p (n=3, L=1)

Triplet Emitter

Electron Configuration of Iridium and Platinum.

Iridium

Ir

(Xe) $4f^{14}$ $5d^{7}$ $6s^{2}$

Z = 77

Platinum

Pt

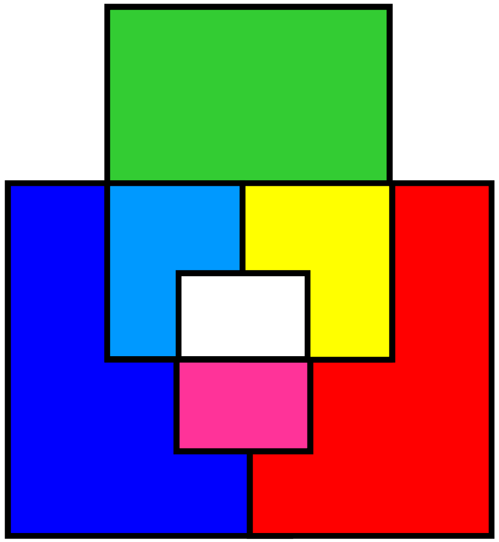
(Xe) $4f^{14}$ $5d^{9}$ $6s^{1}$

Z = 78

Electrons with high orbital angular momentum.

N-Heterocyclic Compounds for OLEDs

Additive Color Mixing

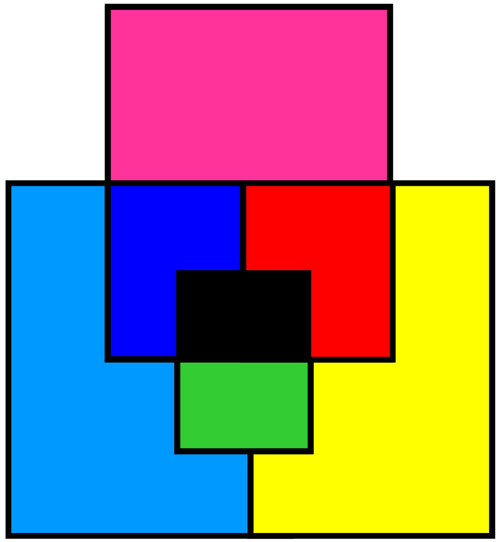


Simultaneous superimposition from light waves of different colors at one and the same place.

Examples:
Color television, color projectors, light-emitting diodes.

Red + **Blue** + **Green** → **White**

Subtractive Color Mixing



Selective fade out / absorption of different colored light waves at one and the same place.

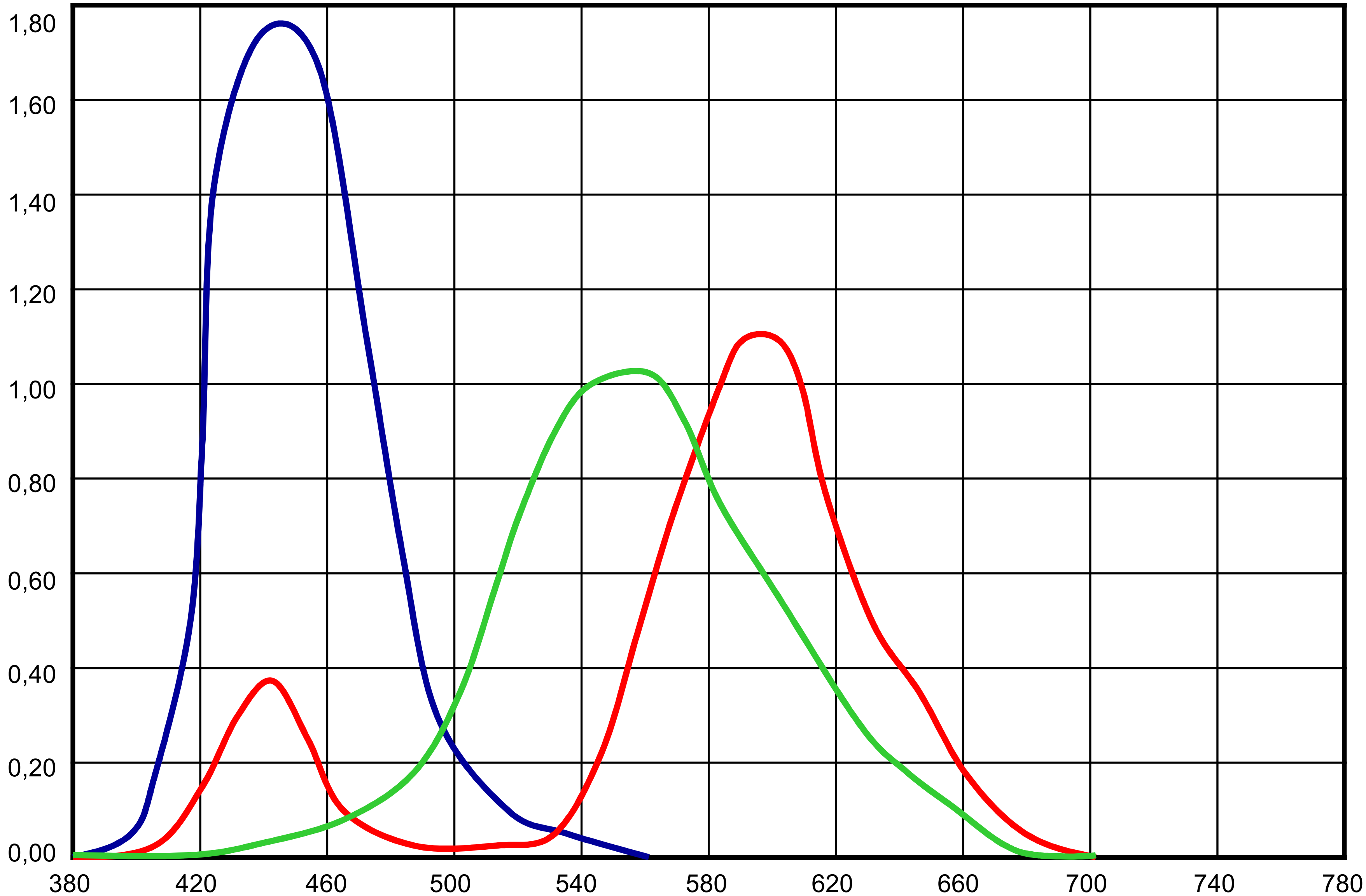
Examples:
Color filters connected in series, mixture of color pigments.

Purpie + **Cyan** + **Yellow** → **Black**

Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

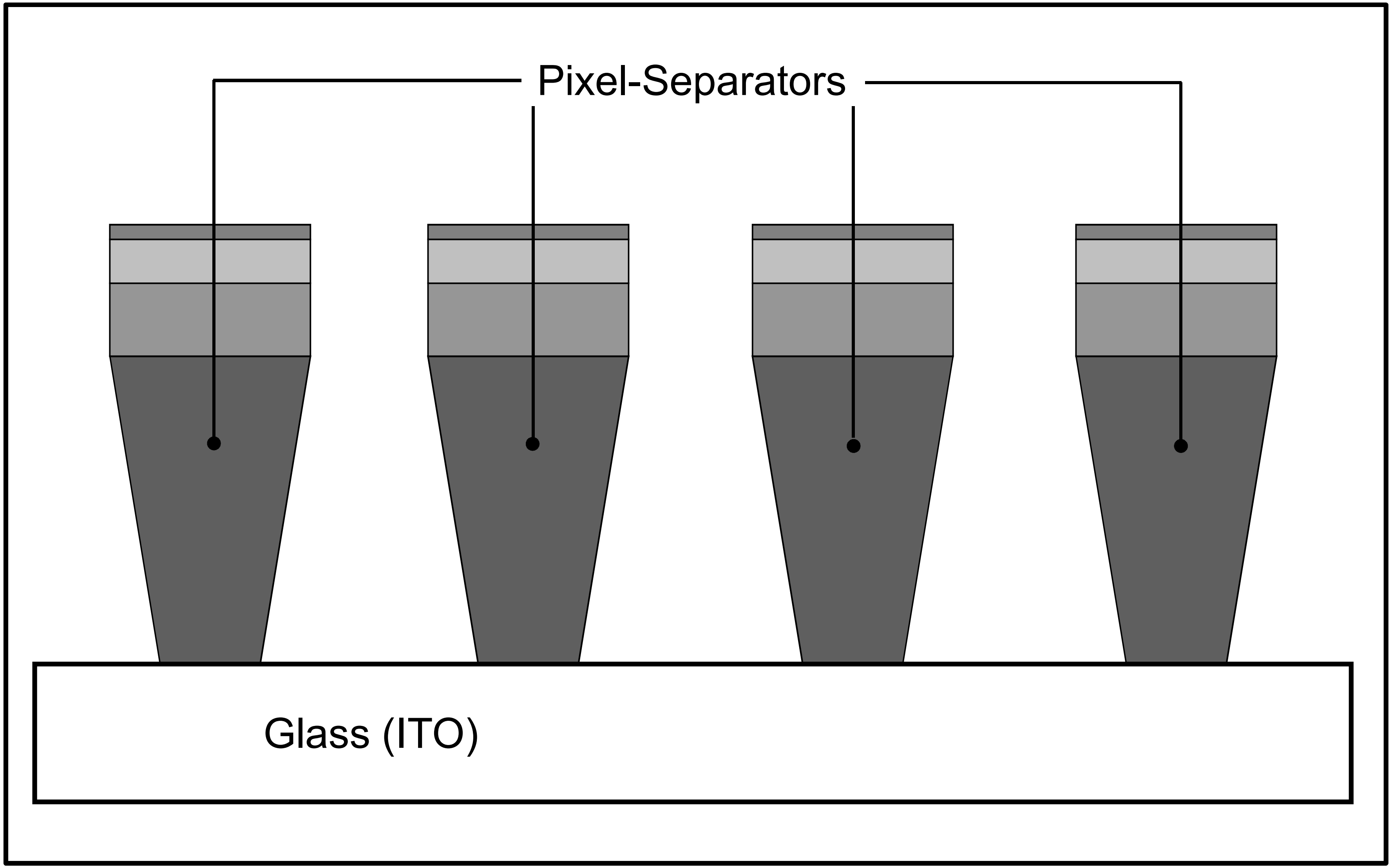
Normalized Responsivity Spectra of Human Cone Cells.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

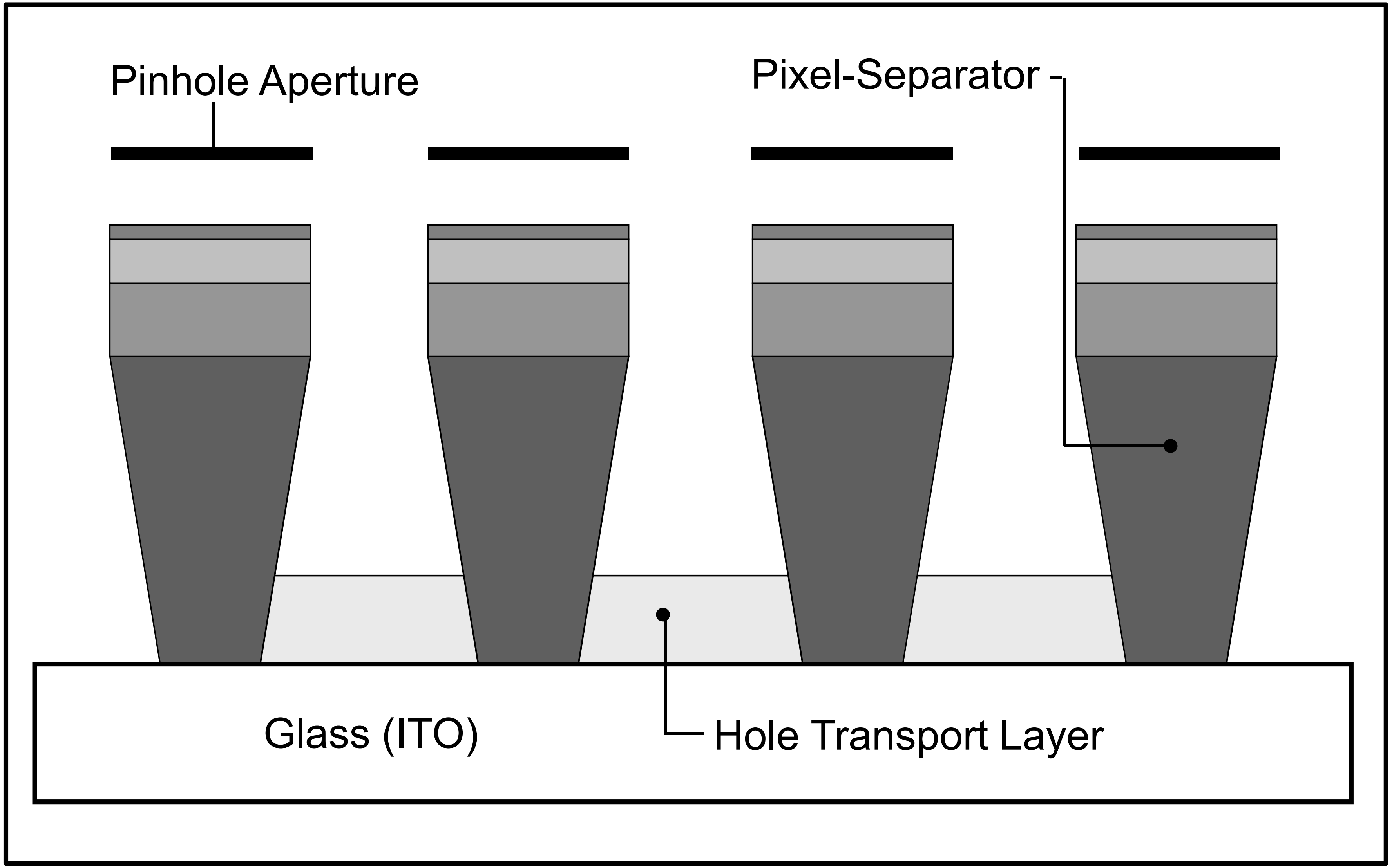
Structuring and Manufacturing of Diode Displays.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

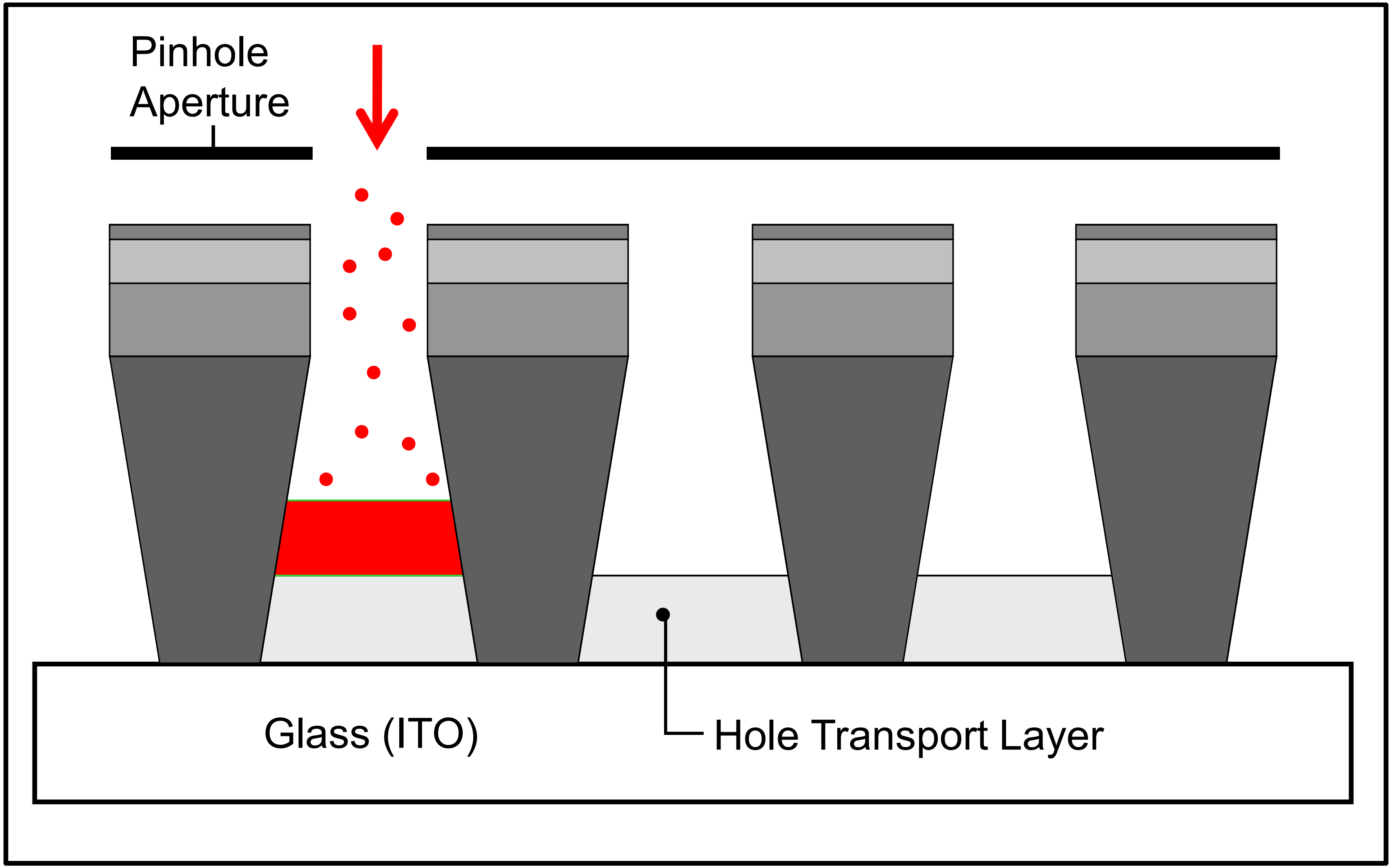
Structuring and Manufacturing of Diode Displays.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

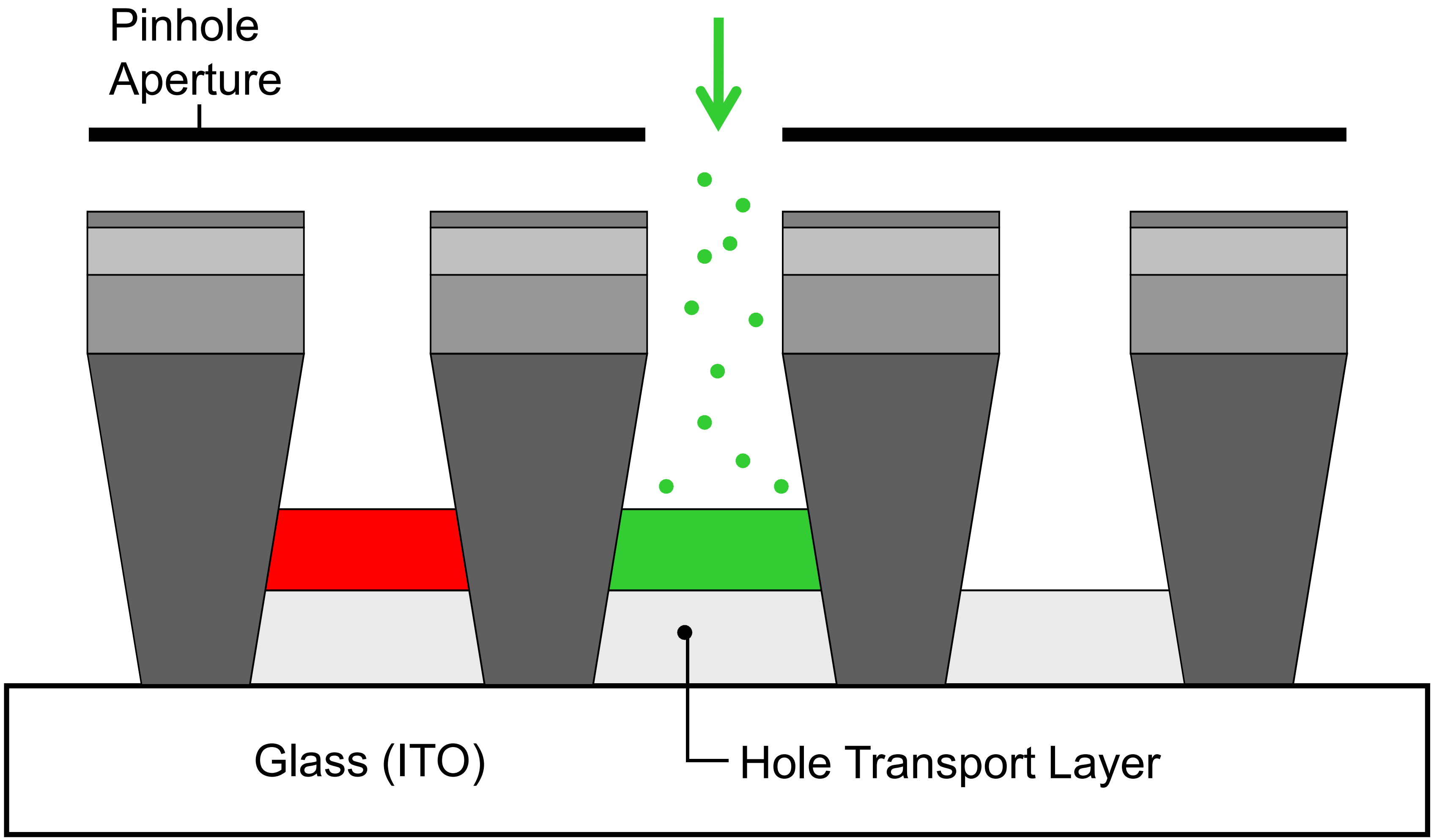
Structuring and Manufacturing of Diode Displays (Piezo Inkjet).



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

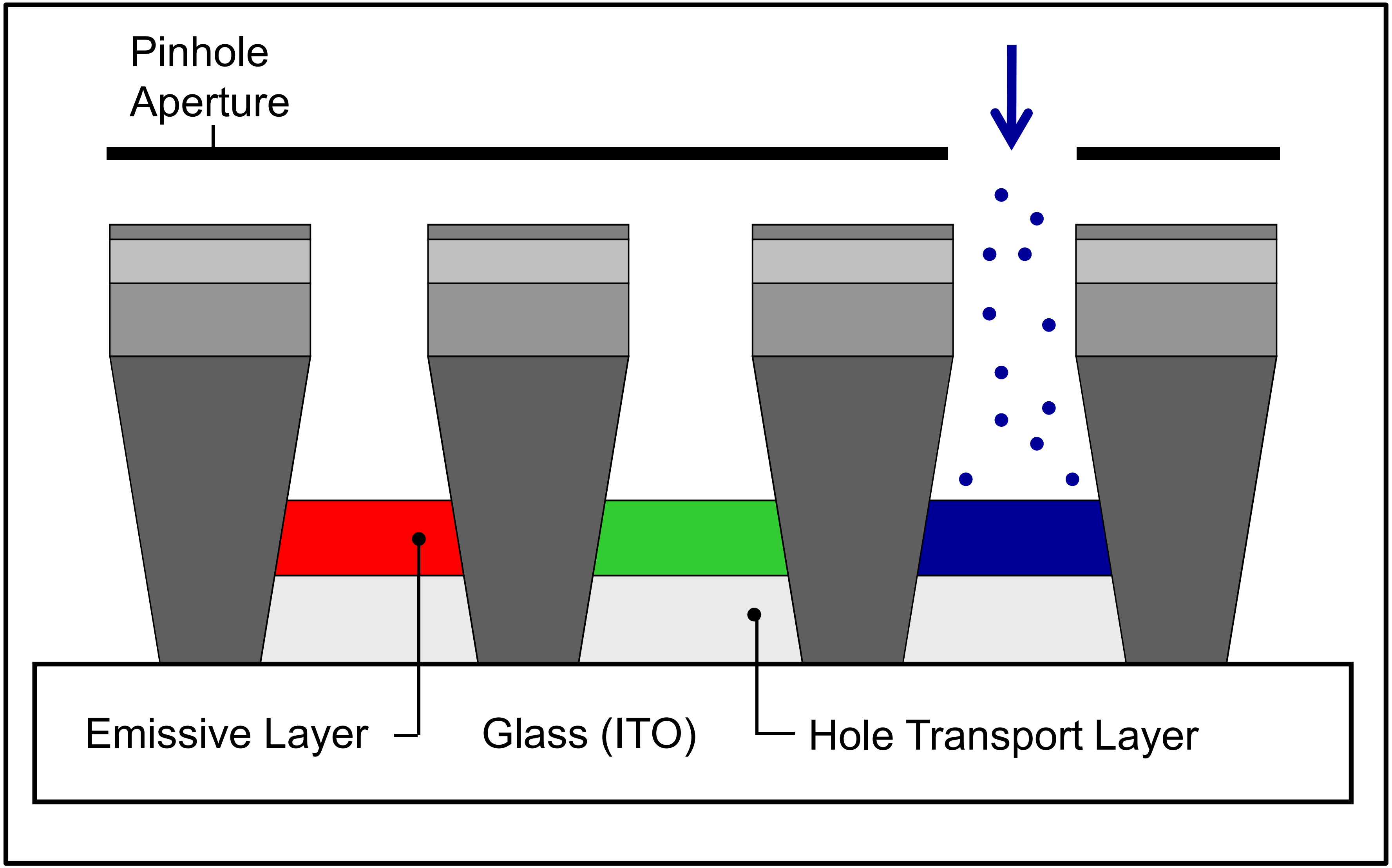
Structuring and Manufacturing of Diode Displays (Piezo Inkjet).



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

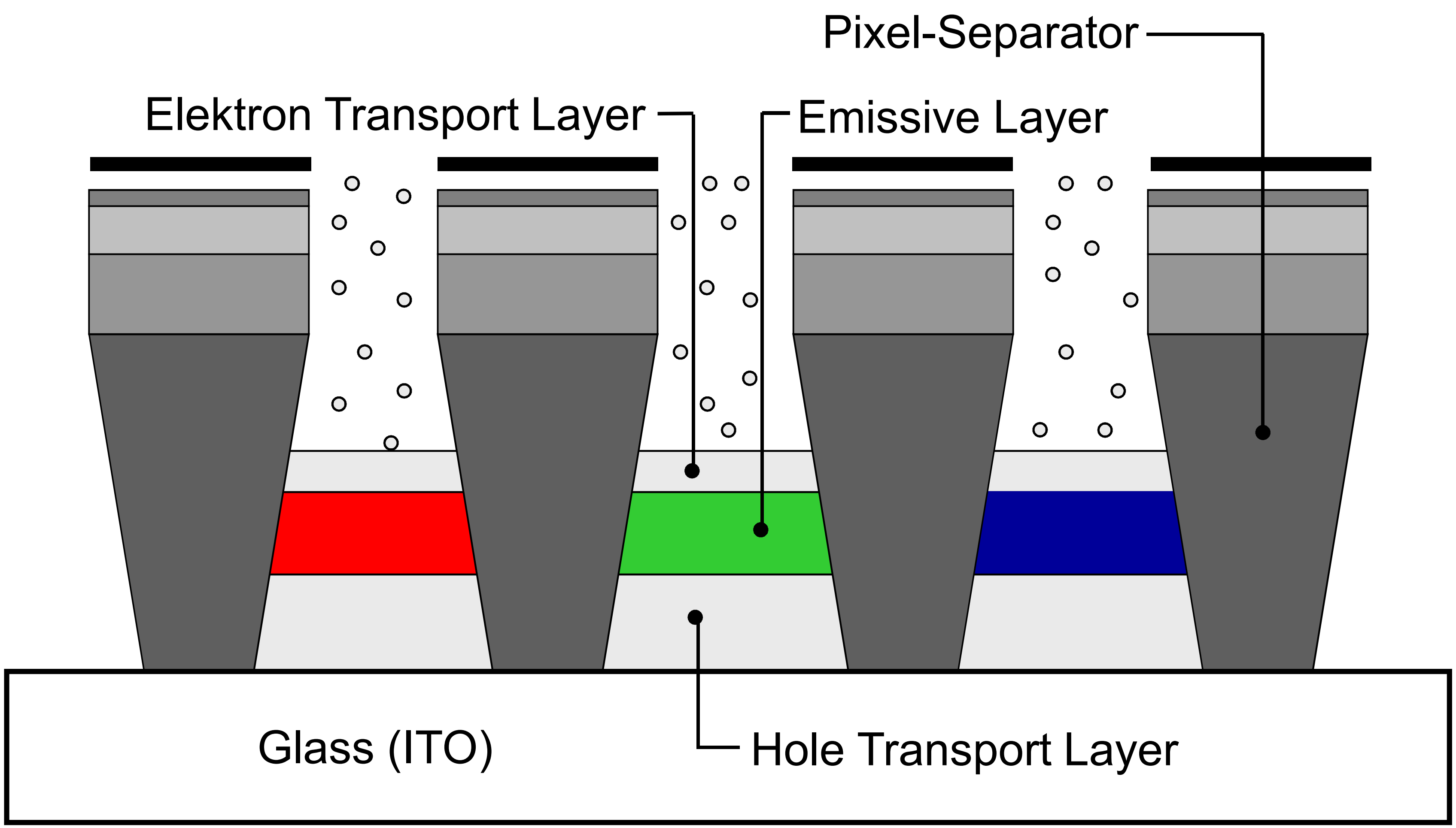
Structuring and Manufacturing of Diode Displays (Piezo Inkjet).



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

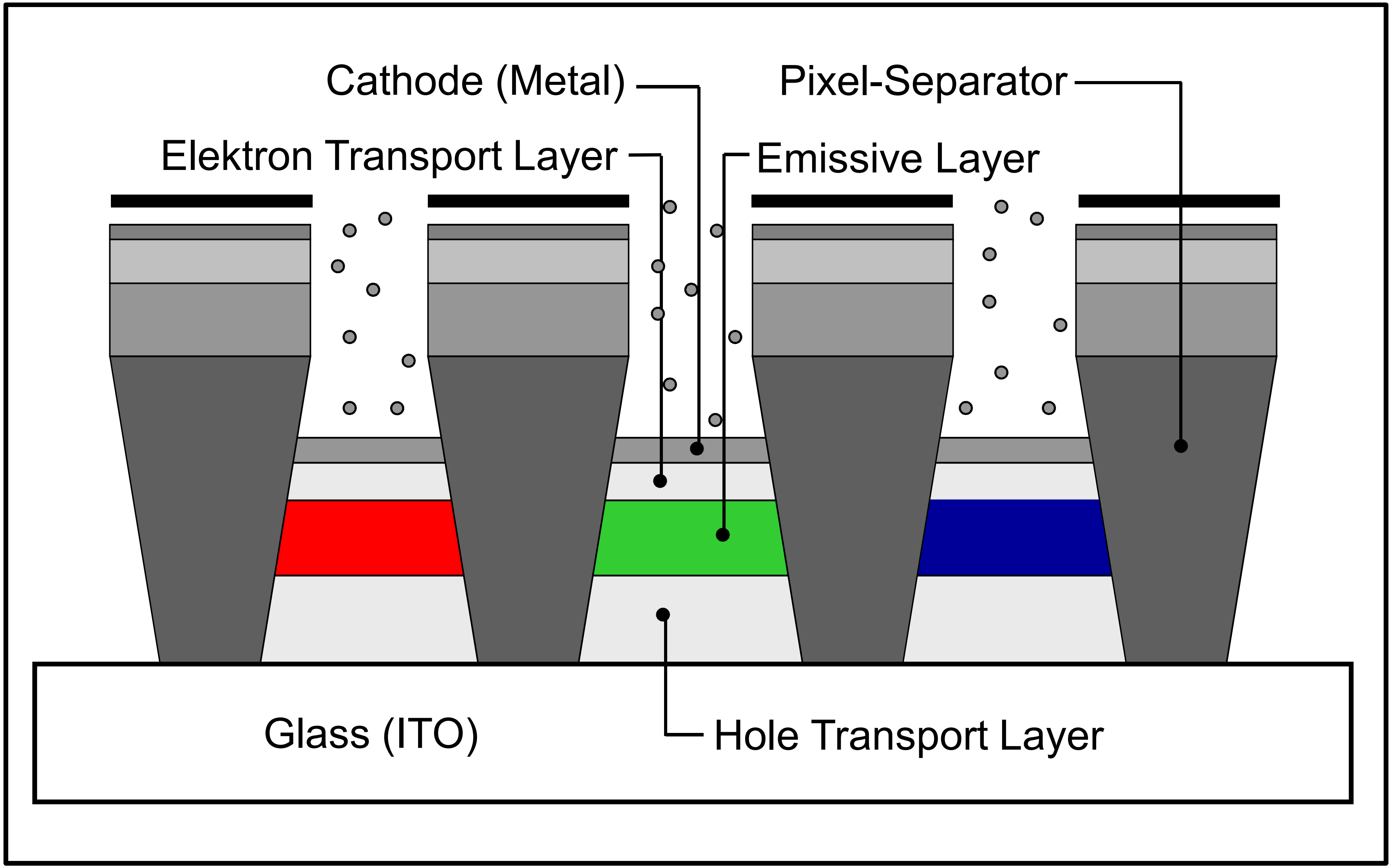
Structuring and Manufacturing of Diode Displays.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

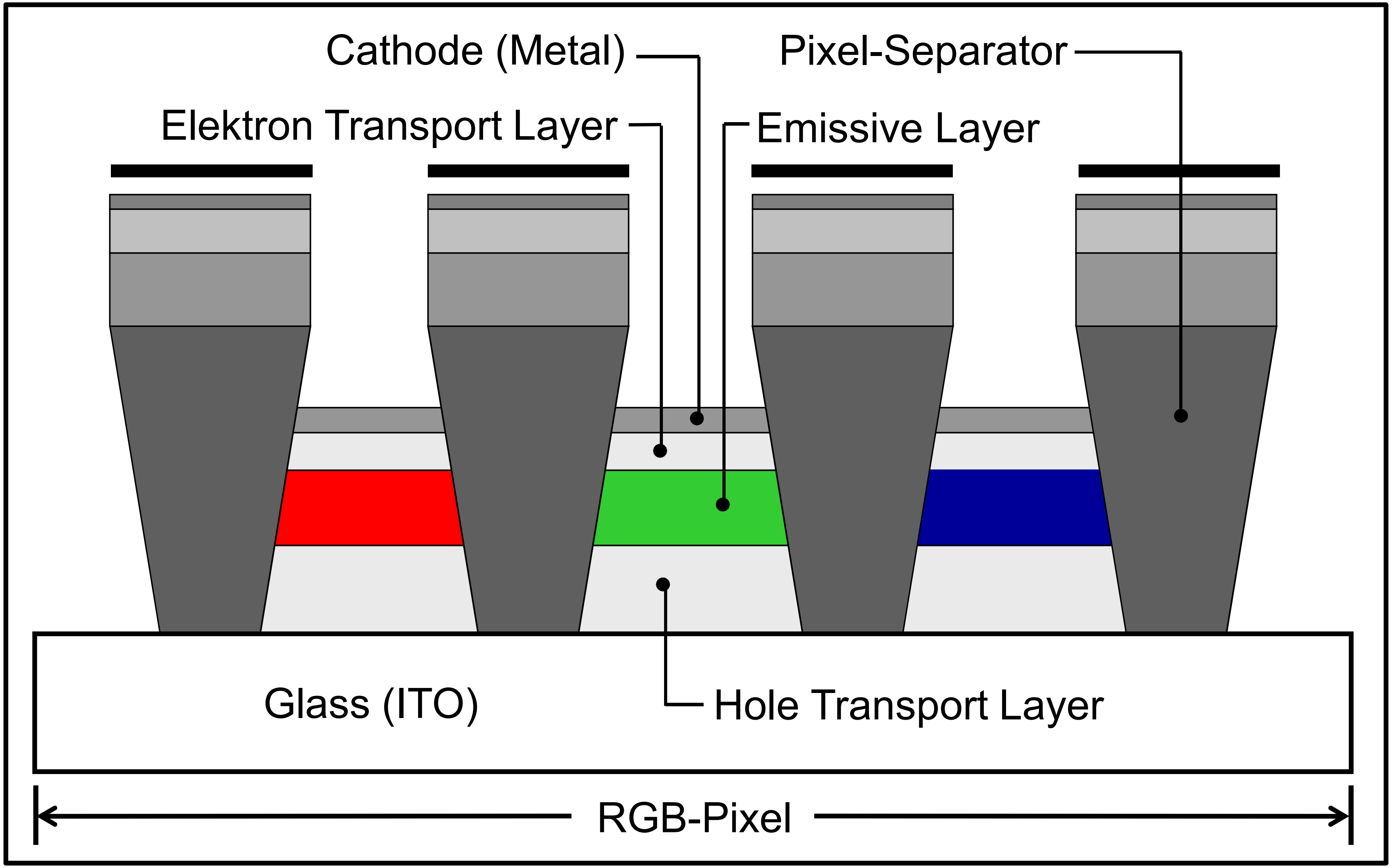
Structuring and Manufacturing of Diode Displays.



Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

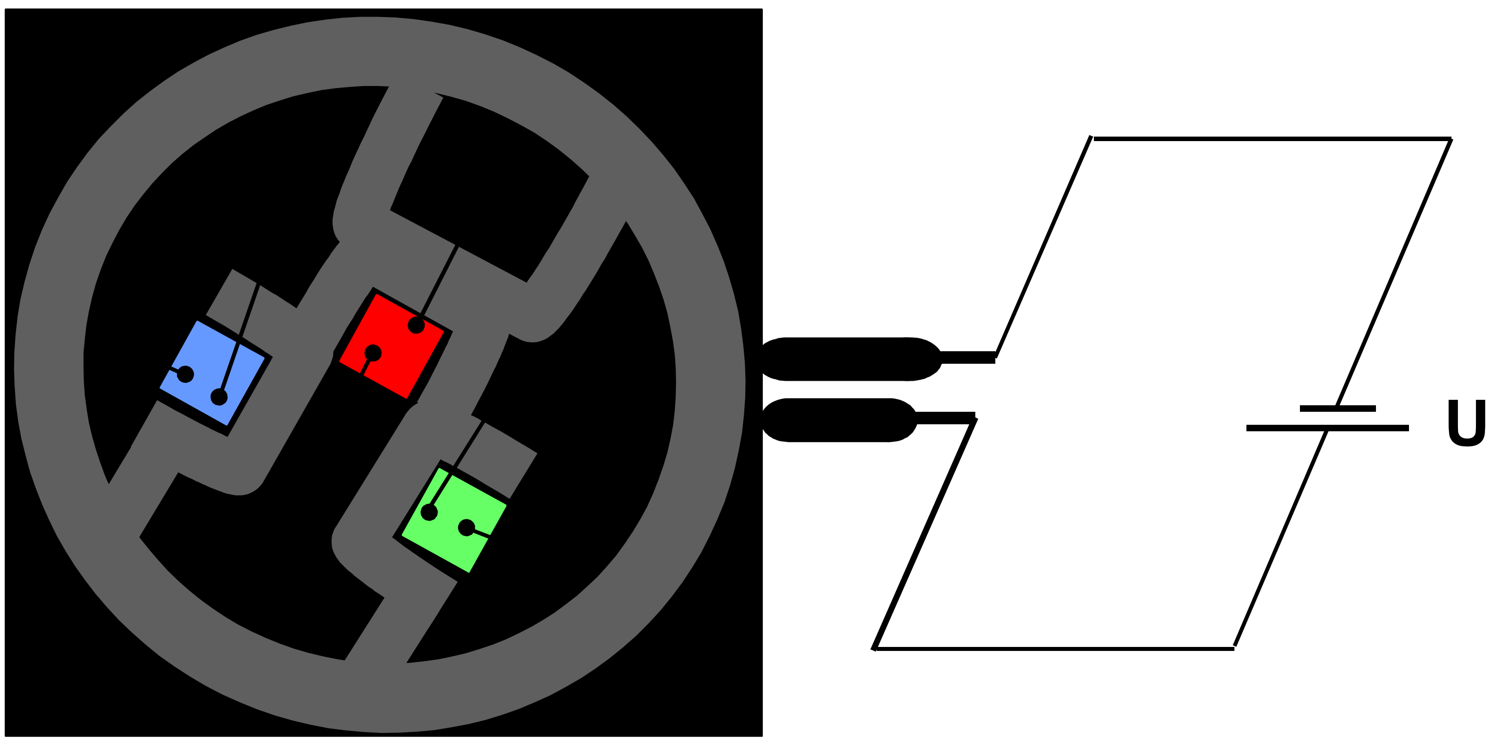
Structuring and Manufacturing of Diode Displays.



Rainer Buerstinghaus

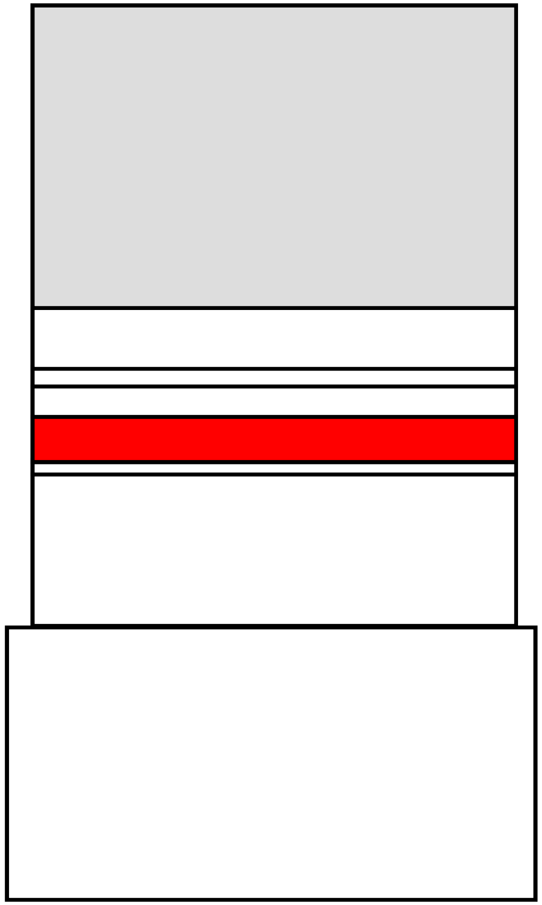
N-Heterocyclic Compounds for OLEDs

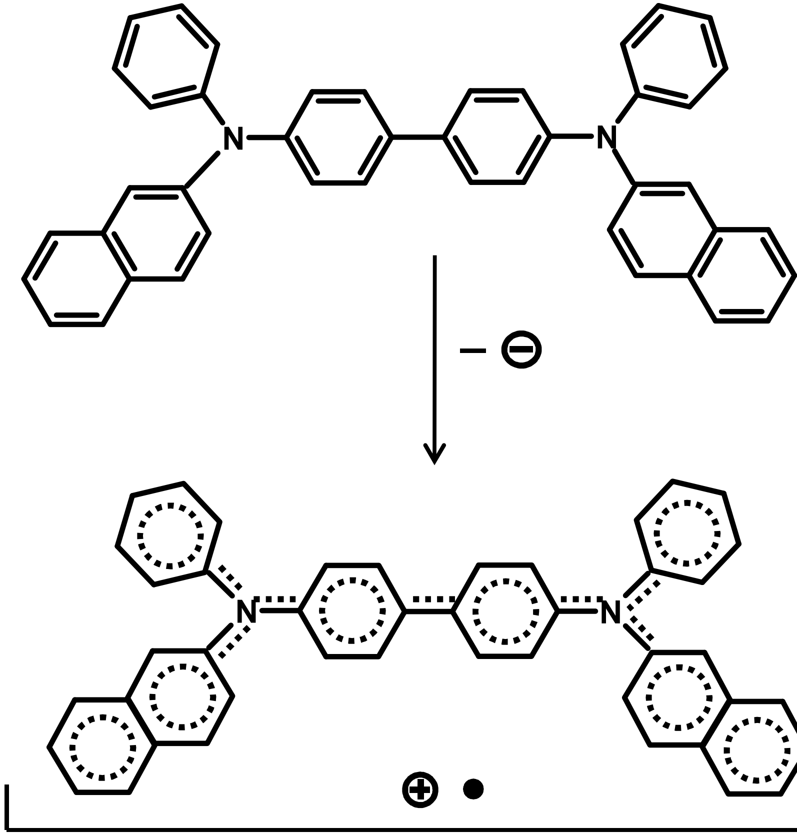
Red-Green-Blue-LED (RGB-LED, Sketch).



Rainer Buerstinghaus

Organic Hole Transport Layer;
Triphenylamine Derivative as a Structural Example, e$^{\ominus}$-Loss.

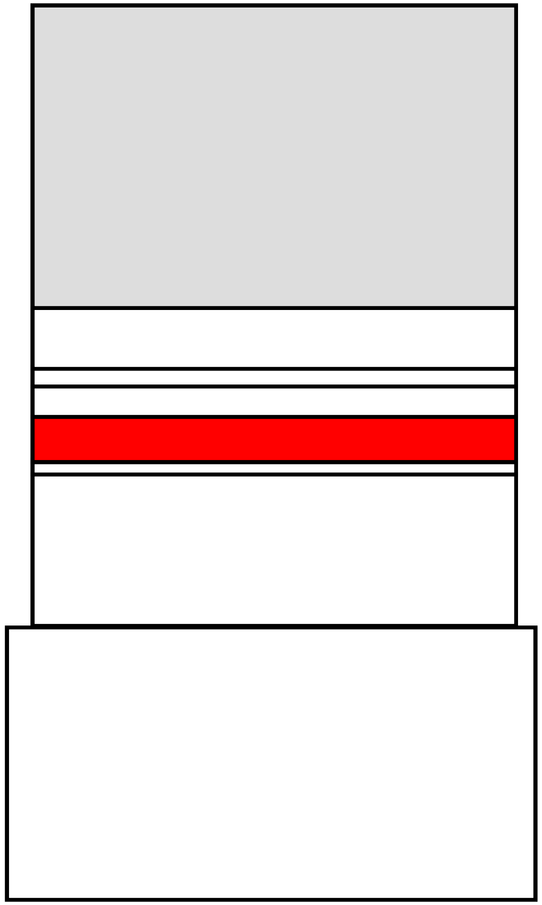


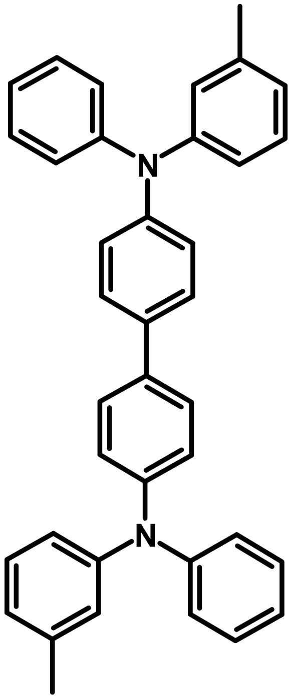


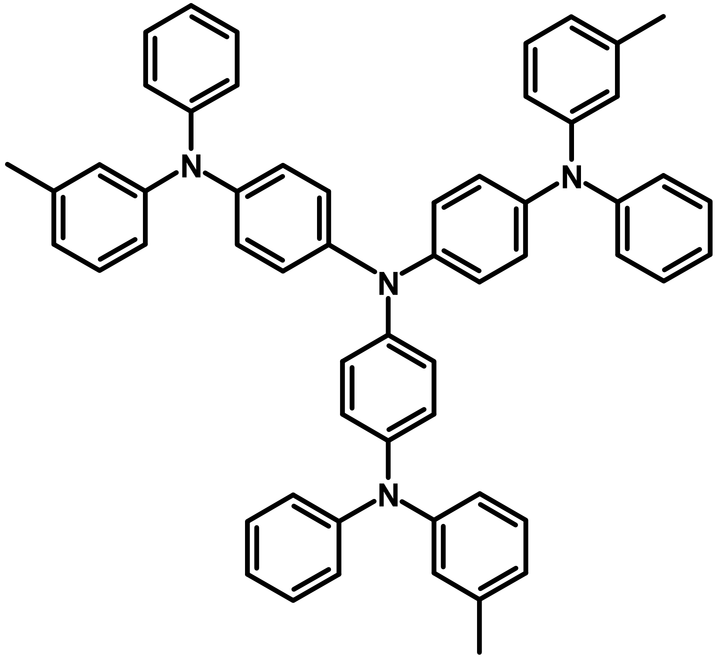
Rainer Buerstinghaus

N-Heterocyclic Compounds for OLEDs

Organic Hole Transport Layer;
Triphenylamine Derivatives, Two Further Structural Examples.

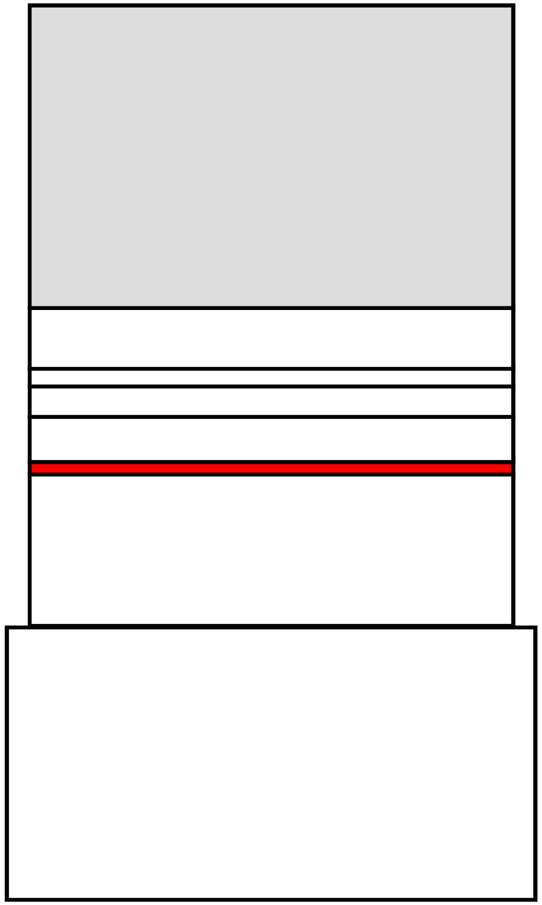


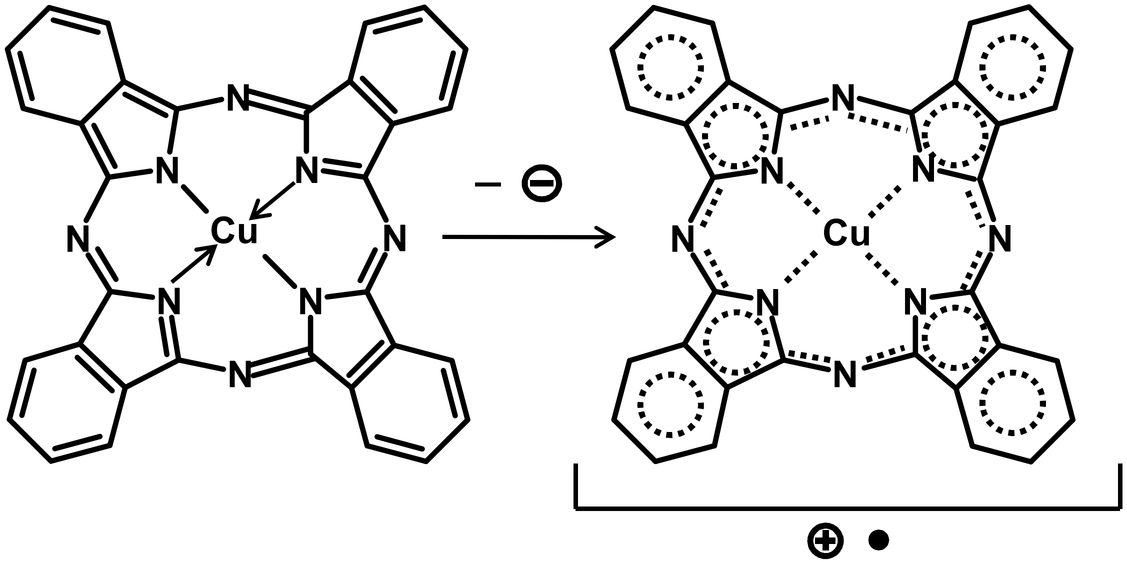




Rainer Buerstinghaus

Organometallic Hole Injection Layer;
Structural Example: Copper Phthalocyanine.

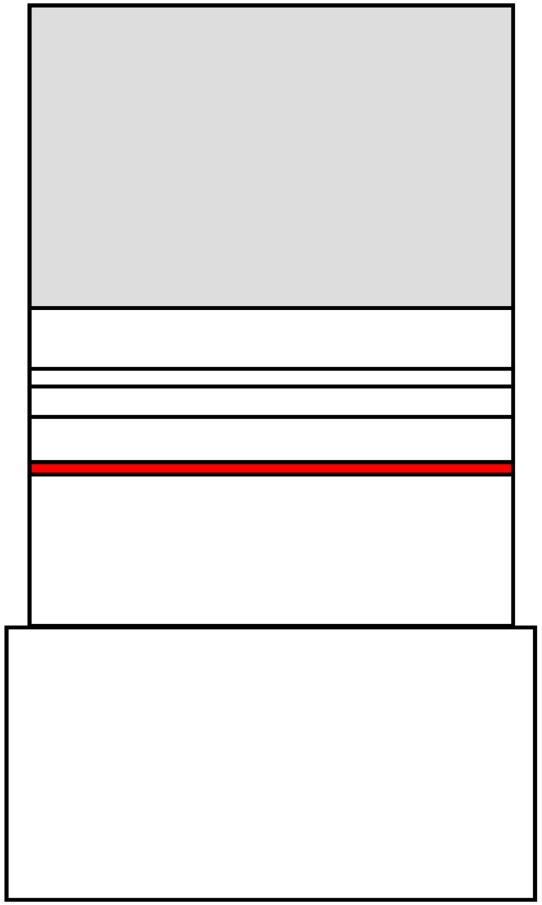


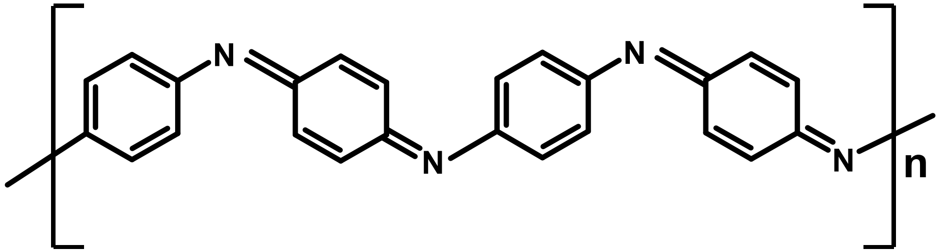


Rainer Buerstinghaus

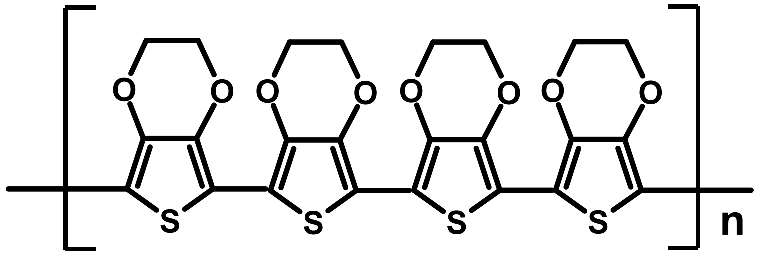
N-Heterocyclic Compounds for OLEDs

Organic Hole Injection Layer; Other Non-Metallic, Polymeric Conductors.





PANI: Polyaniline



PEDOT: Polyethylene Dioxythiophene

Rainer Buerstinghaus

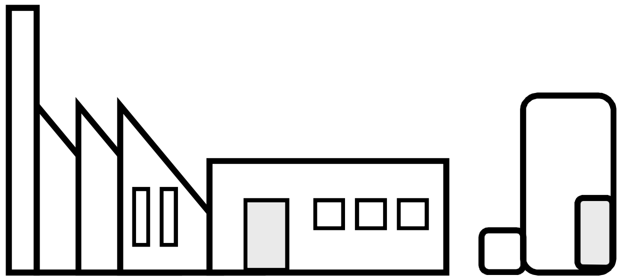
Task for a Case Study on R&D Project Management !

Plan a suitable project for your research subject:
"N-Heterocycles for Emitter Layers in OLEDs"!

- General Framework: The R&D project to be planned should be of strategic importance for your (start-up) company or institute for applied research!
- Define from your sight, what you consider to be a plausible target system for this R&D project: chemical-technical, economic and time objectives, taking into account the state of science, the state of the art, the current development of the market and the competition, respectively. Use additional data and facts from the Internet/WWW to assess the economic, technical and social environment!
- Roughly estimate the personnel and material expenses necessary for the complete achievement of the target system!
- Decide on an appropriate project organization!
- Determine the target-relevant tasks and classify these according to the number of specialist functions involved in their solution!
- Based on this, carry out a rough project structure planning (sketch)!
- Create a first, simple project phase plan by using bars on time axes for this according to the technique of Henry Gantt!
- Make a plausible SWOT analysis for this research project!

Task for a Case Study on R&D Project Management

N-Heterocycles for Emitter Layers in OLEDs.



The Chemical Company "[…GmbH5]" :

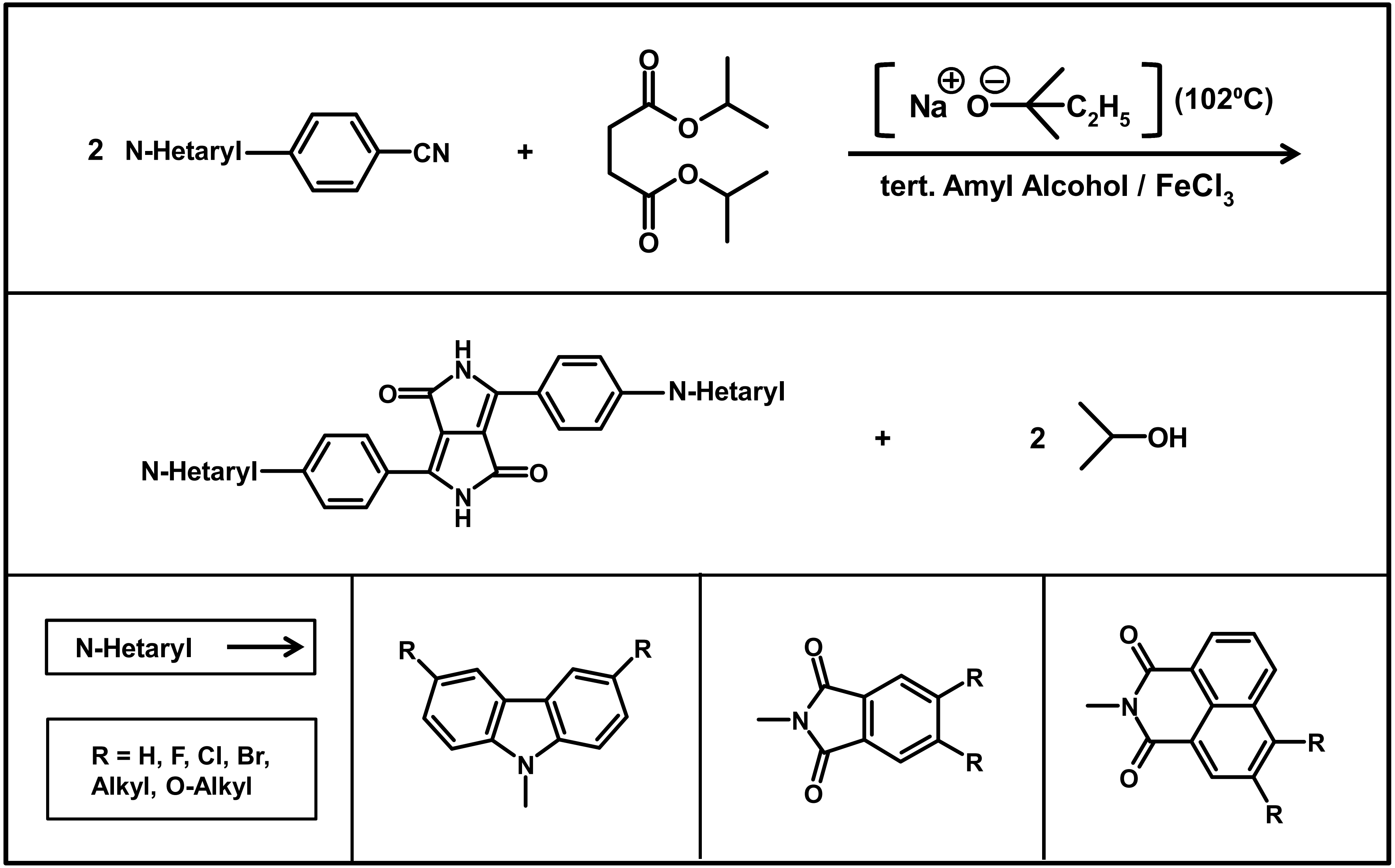
Medium-sized company, 840 employees, including 35 chemists,
47 engineers (FH), 19 engineers (TU).

Own research and development, own production.

Active in the field of chemicals for organic light-emitting diodes for 7 years.
Chemical specialty: N-heterocyclic compounds.

Task for a Case Study on R&D Project Management

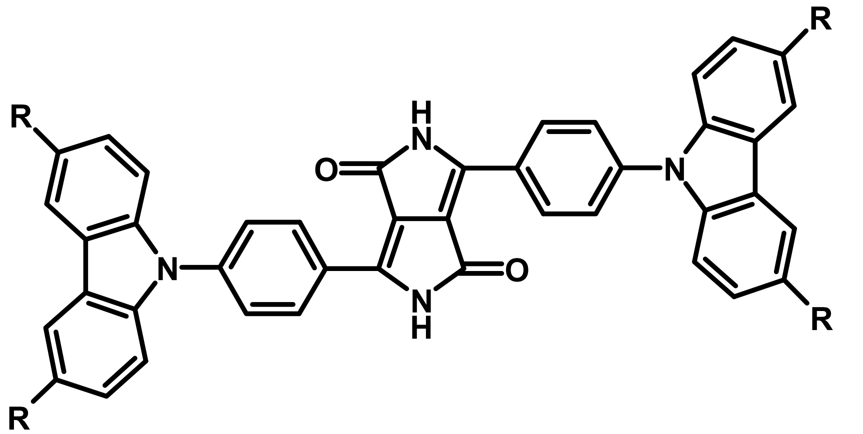
Stobbe Condensation of N-Hetaryl-Substituted Benzonitriles.



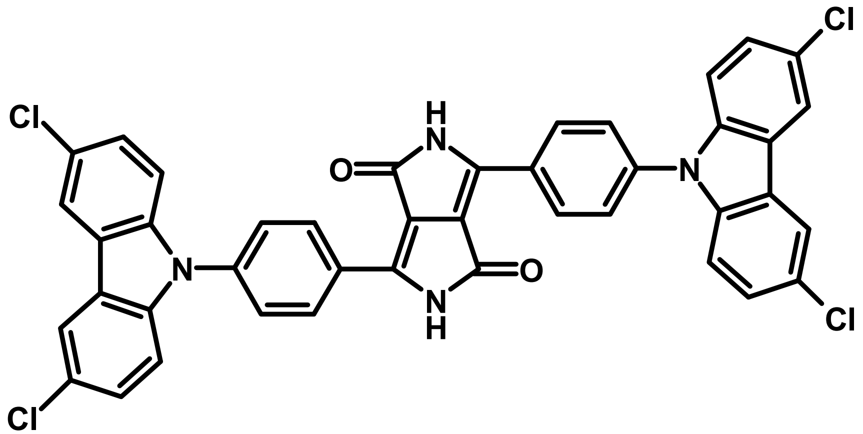
Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

Target Structures in the First Laboratory Syntheses, Examples.



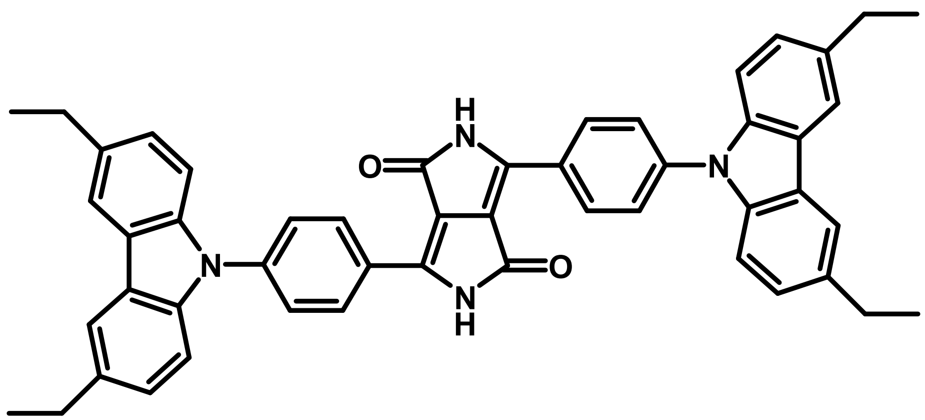
With R = H, F, Cl, Br, Alkyl, O-Alkyl

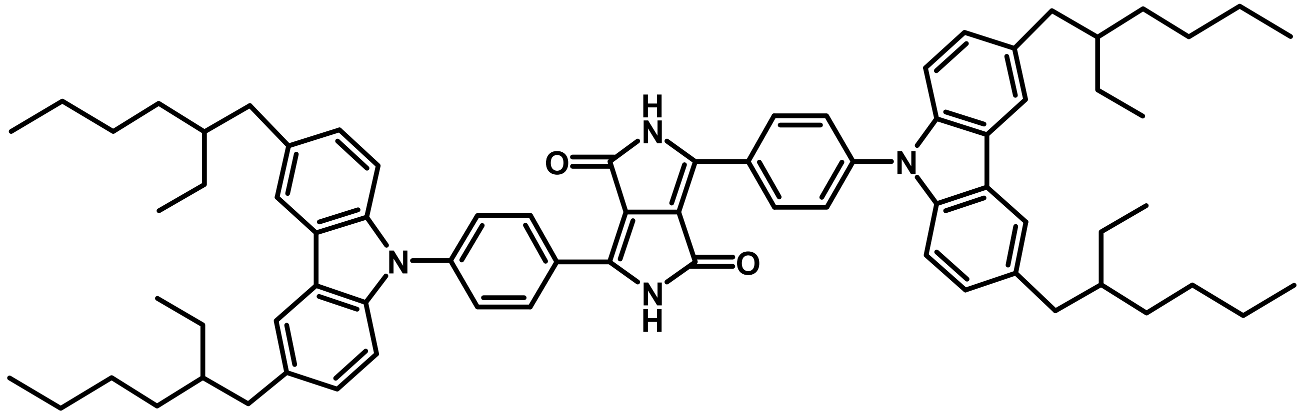


Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

Target Structures in the First Laboratory Syntheses, Examples.

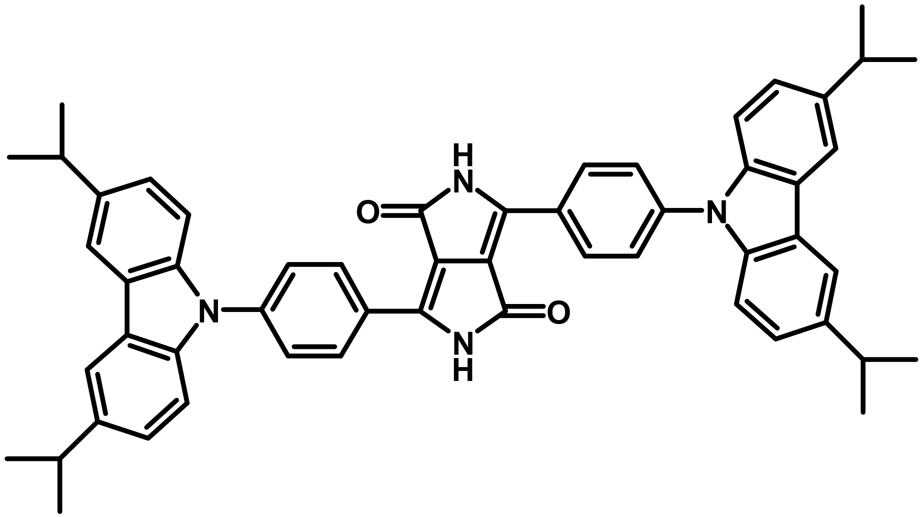


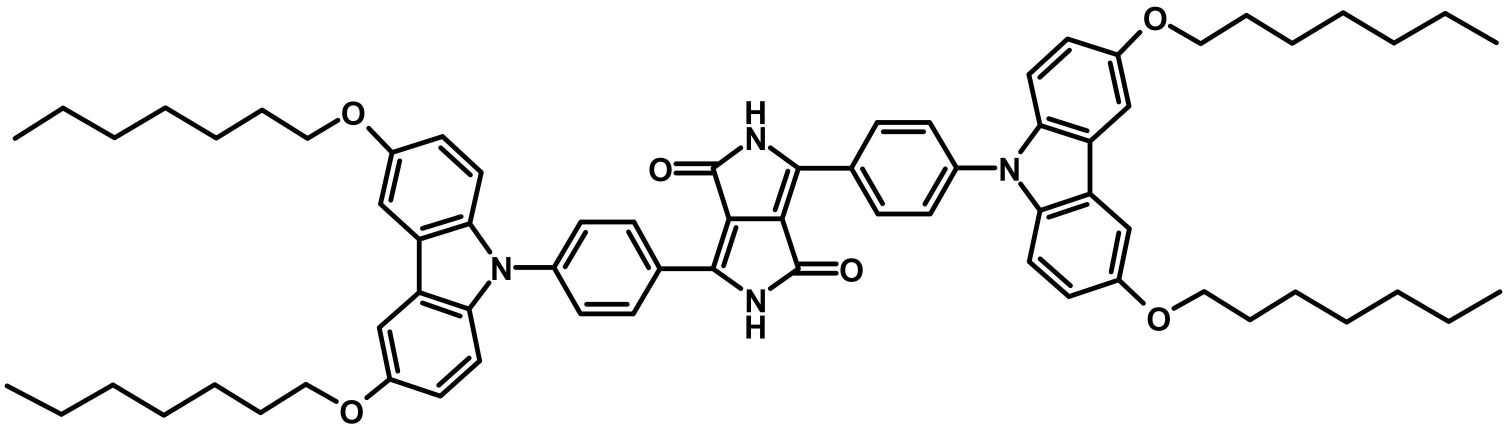


Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

Target Structures in the First Laboratory Syntheses, Examples.

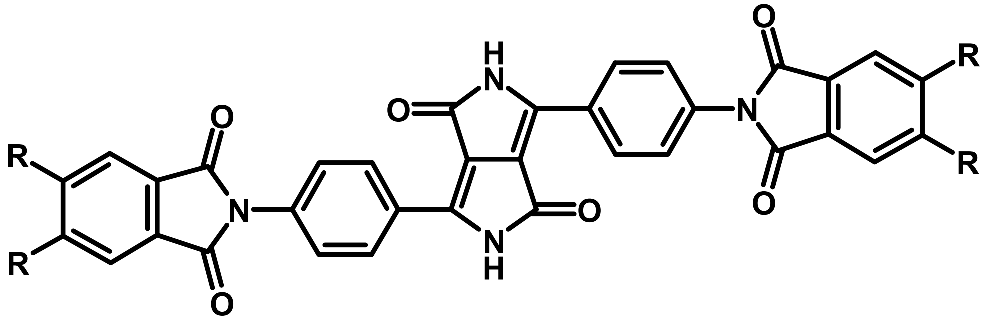




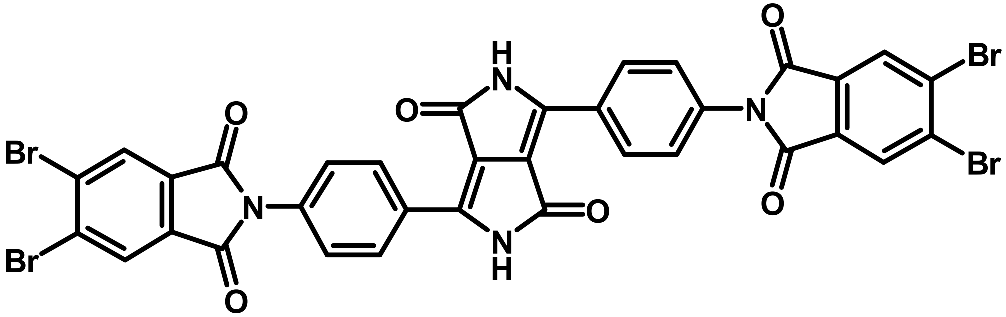
Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

Target Structures in the First Laboratory Syntheses, Examples.



With R = H, F, Cl, Br, Alkyl, O-Alkyl

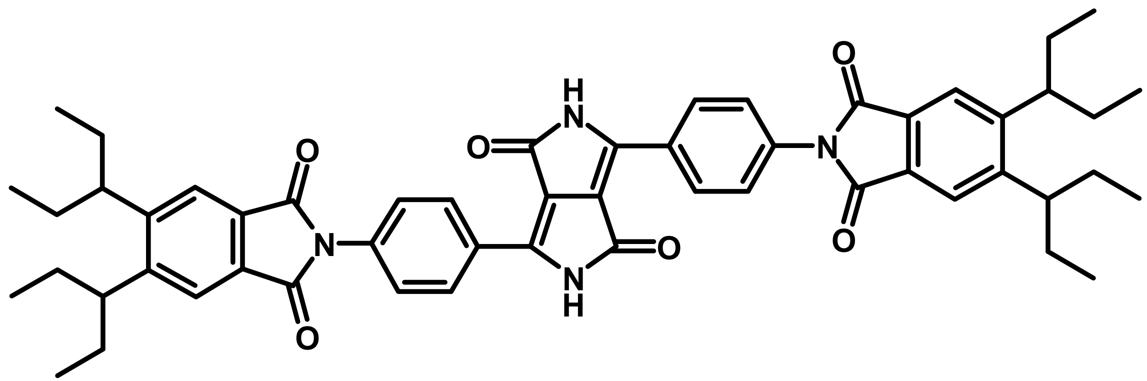


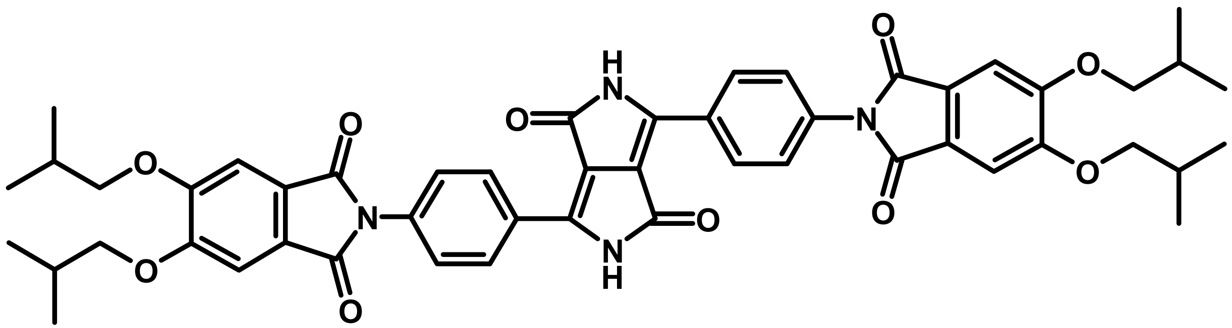
Instead of Bromine: Fluorine or Chlorine

Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

Target Structures in the First Laboratory Syntheses, Examples.

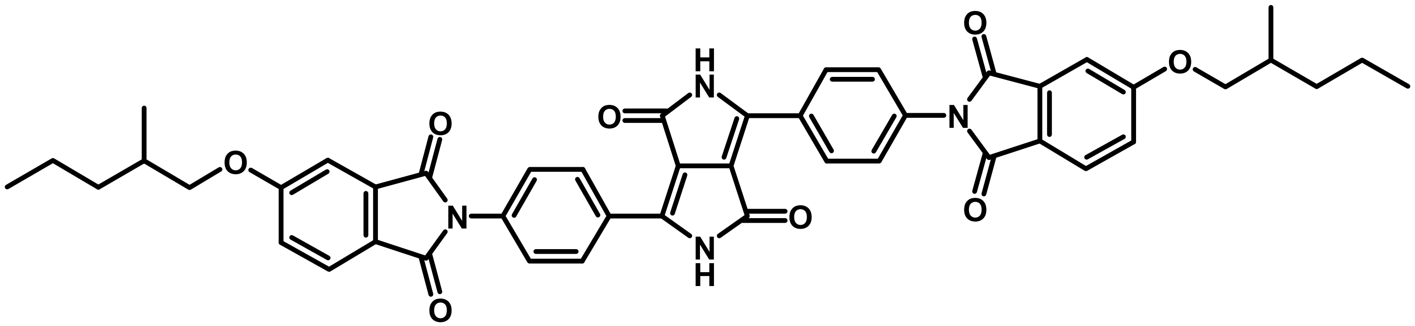


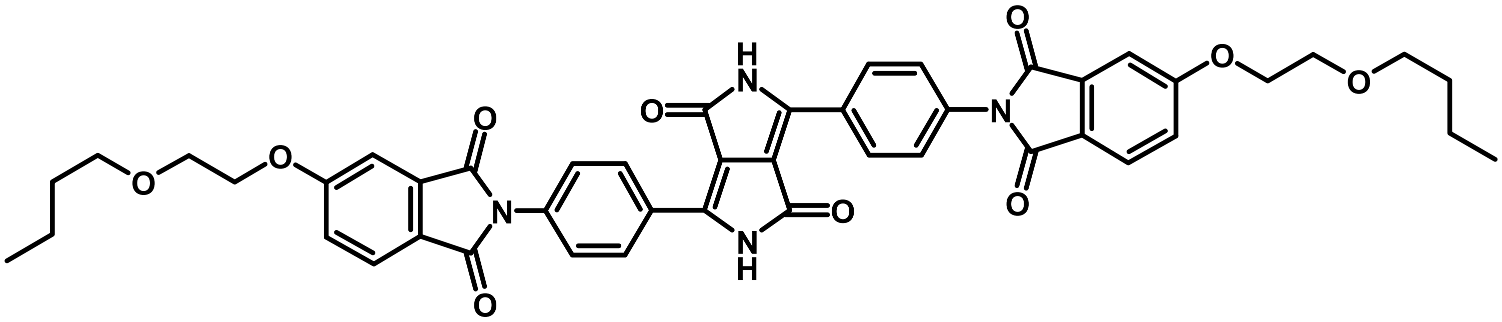


Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

Target Structures in the First Laboratory Syntheses, Examples.

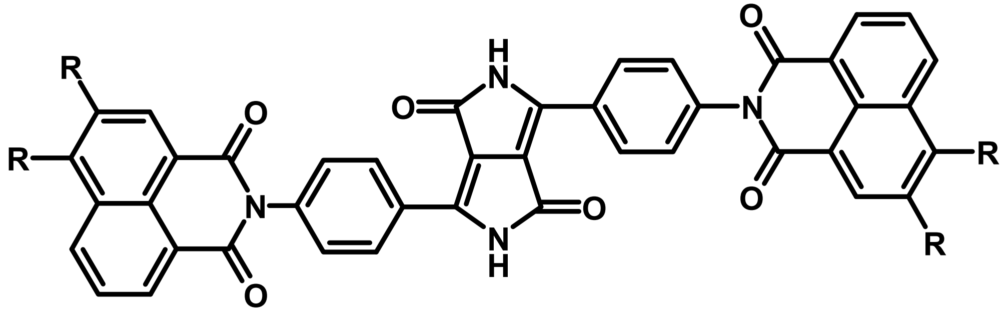




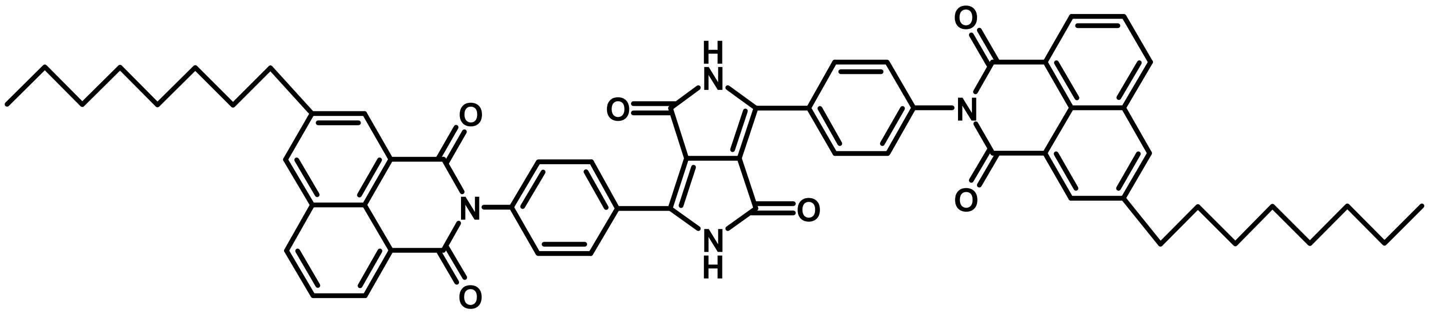
Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

Target Structures in the First Laboratory Syntheses, Examples.



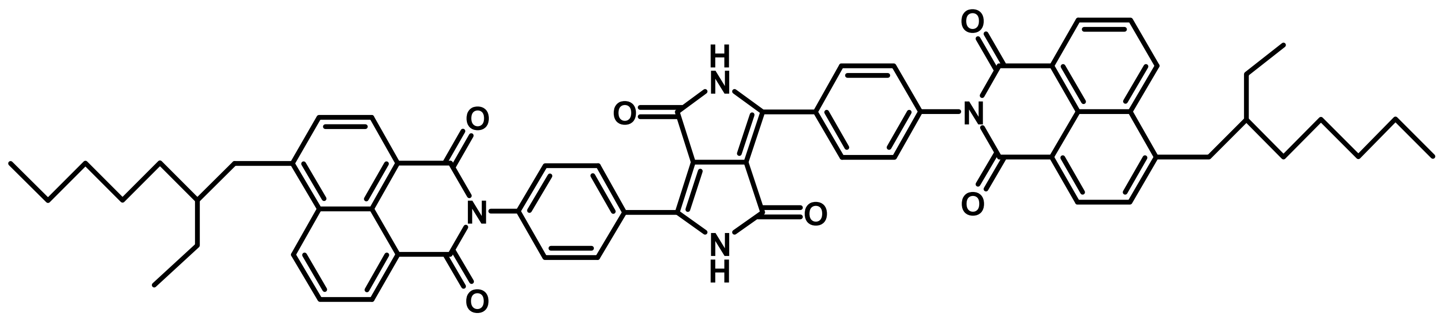
With R = H, F, Cl, Br, Alkyl, O-Alkyl

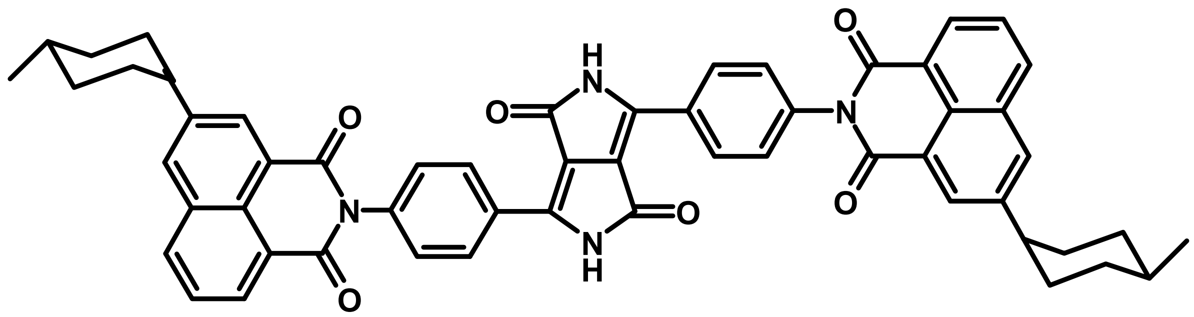


Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

Target Structures in the First Laboratory Syntheses, Examples.

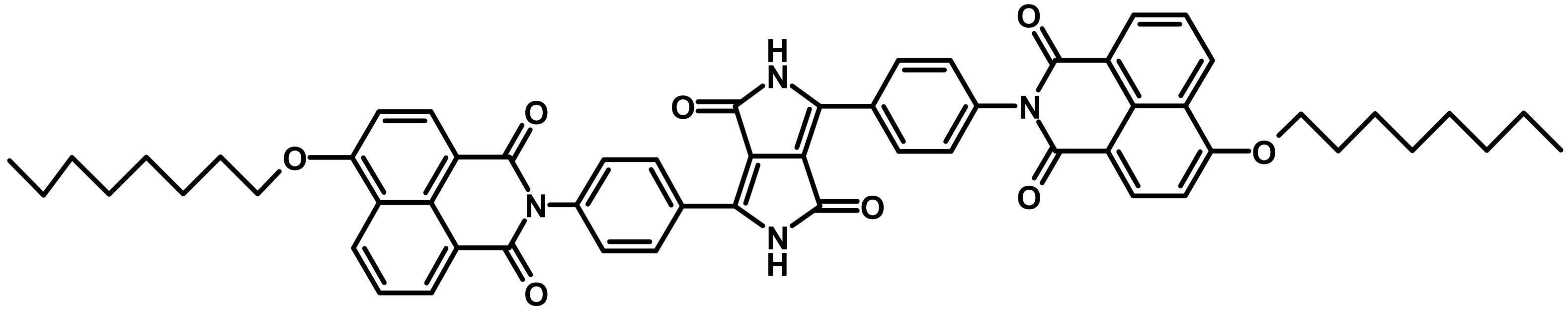


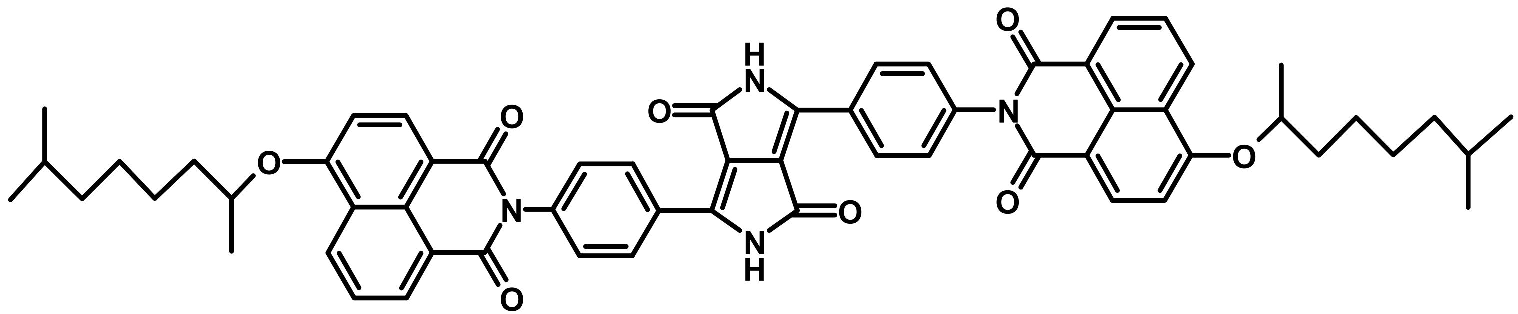


Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

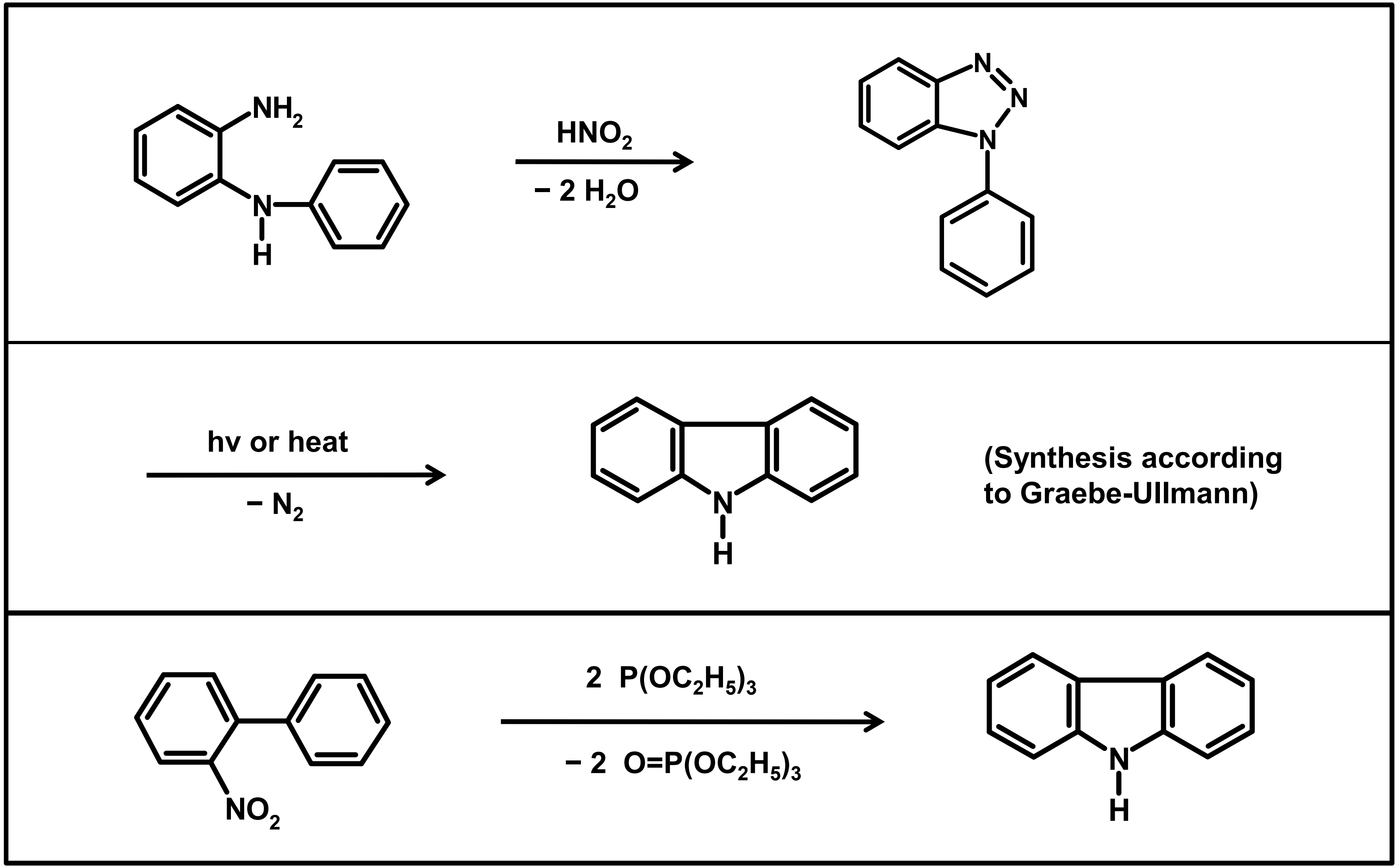
Target Structures in the First Laboratory Syntheses, Examples.





Task for a Case Study on R&D Project Management

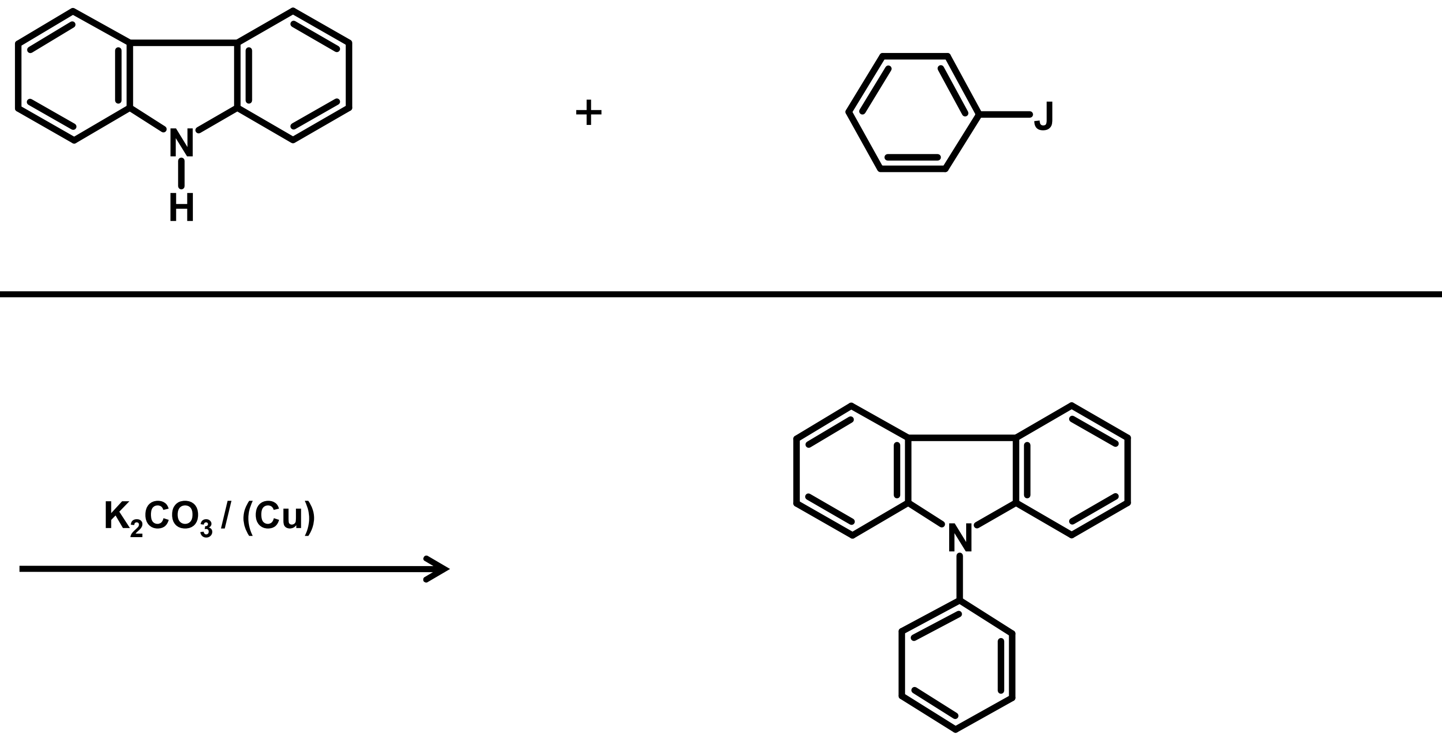
Carbazole Syntheses (Graebe Ullmann; Reductive Ryclization).



Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

Synthesis of N-Phenylcarbazole According to Ullmann.



Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

Applications of Organic Light-Emitting Diodes, 2020.

General Light Sources	"Light Windows"
Designer Lamps	Background for LCDs
All Kinds of Touchscreens	Advertising Display Boards
Smart TV Screens	PC Monitors
Traffic Markings	Interior Markings

Rainer Buerstinghaus

Task for a Case Study on R&D Project Management

Applications of Organic Light-Emitting Diodes, 2020.

Displays: Roll-up Sets	Displays: Wearable Devices
Displays: Game Consoles	Displays: Electrical Appliances
Displays: Notebooks	Displays: Broadcast Receivers
Displays: Smartphones	Displays: iPads
Displays: Digital Cameras	Displays: MP3-Players

Task for a Case Study on R&D Project Management

Physical Profile of Requirements for OLEDs, 2020.

Physical Parameters 2020	
Panel Efficiency	140 lm/W
Illuminance	> 15.000 cd/m^2
Lumen-Output	> 40.000 lm/m^2
Color Rendering Index, CRI	> 95 %
Technical Lifetime at 3000 cd/m^2	> 40.000 h
Maximum Size	500 x 500 mm^2

Task for a Case Study on R&D Project Management

Development of the Areal Applications of OLEDs.

Year	Areal Application
2007	Small Displays
2008	Medium and Large Displays
2010	Lighting Purposes
2012	Flexible Decorative Lights
From 2020	Large Display Boards

Task for a Case Study on R&D Project Management

Worldwide Turnover of Organic Light Emitting Diodes.
(2020-2023: Forecasts)

Year	Turnover (Billions €)	Growth Over the Previous Year
2014	07,9	–
2015	12,0	51,8 %
2016	15,5	29,2 %
2017	19,0	22,6 %
2018	25,0	31,6 %
2019	30,0	20,0 %
2020	35,0	16,7 %
2021	39,2	12,0 %
2022	41,8	06,6 %
2023	44,4	06,2 %

Task for a Case Study on R&D Project Management

Scenario 2025 from "Market Technology Analysts".

- Every third light source is an LED.
- Power consumption, worldwide: − 10%.
- Electricity costs reduced by € 100 billion every year.
- 50 billion euros less investment costs for power plants.
- Cars with combustion engines:
  Reduction of fuel consumption by 0.2 liters per 100 km with white LEDs.

Task for a Case Study on R&D Project Management

Principal Producers of OLED Displays, Worldwide, 2020.

Company	Country
AU Optronics	TWN
BOE Display	CHN
China Star Optoelectronics Technology	CHN
eMagin Corporation	USA
EverDisplay Optronics	CHN
Guangzhou New Vision Optoelectronics	CHN
Innolux	TWN
Japan Display	JPN
Kopin	USA
Kunetech	–

Task for a Case Study on R&D Project Management

Principal Producers of OLED Displays, Worldwide, 2020.

Company	**Country**
Kyocera Display	JPN
LG Display	KOR
MicroOled	GER
Nippon Seki	JPN
Oasis New Energy	CHN
OLiGHTEK	CHN
Pioneer	JPN
RiT Display	TWN
Royole	CHN
Samsung Display	KOR

Task for a Case Study on R&D Project Management

Principal Producers of OLED Displays, Worldwide, 2020.

Company	Country
Seeya Technology	CHN
Sharp	JPN
Sichuan CCO	CHN
Sony	JPN
Tianma	CHN
Truly Semiconductors	HKG
Visionox	CHN
Winstar	TWN
Wintek	TWN
WiseChip	TWN

Further literature (specialist books, specialist articles) on the subject: "N-Heterocyclic Compounds for Organic Light-Emitting Diodes, OLEDs".

- W. E. Howard: Better displays with organic films, Scientific American. 290, Nr. 2, 2004, 76–81.
- D. Hertel, C.D. Müller, K. Meerholz, Chemie in unserer Zeit 2005, 336.
- H. Yersin, Highly Efficient OLEDs with Phosphorescent Materials, Wiley-VCH, Berlin, 2007.
- B. E. A. Saleh, M. C. Teich, Grundlagen der Photonik, Wiley-VCH, Weinheim, 2008.
- B. Riedel, Effizienzsteigerung in organischen Leuchtdioden, Dissertation, KIT-Scientific Publishing, Karlsruhe 2011.
- Joseph Shinar (Hrsg.): Organic Light-Emitting Devices: A Survey. Springer, New York, 2012.
- T. Tsujimura, OLED Displays, Fundamentals and Applications, J. Wiley & Sons, Hoboken, New Jersey, 2012.
- A. Buckley, Organic Light-Emitting Diodes (OLEDs), Woodhead Publishing, Cambridge, 2013.
- C. Kölper, W. Bergbauer, M. Strassburg, N. Lindner, Physik in unserer Zeit, 2011, 92-98.
- X. Yang, X. Xu, G. Zhou, J. Mater. Chem. C, 2015, 913-944.
- D. Wöhrle, Chemie in unserer Zeit, 2015, 386-401.
- D. Wöhrle, Chemie in unserer Zeit, 2016, 244-259.
- D.J. Gaspar, E. Polikarpov, OLED Fundamentals, Materials, Devices and Processing of Organic Light-Emitting Diodes, CRC Press, Abingdon, U.K., 2015.
- G. Baldcchini, Organometallic Luminescence: A Case Study on Alq3, an OLED Reference Material, Elsevier, Woodhead Publishing, Cambridge 2020.
- M. Koden, OLED Displays and Lighting, J. Wiley & Sons, Chichester, 2017.
- R. Z. Li , Organic Light-Emitting Materials and Devices, CRC Press, Abingdon, U.K., 2017.
- P. A. Tipler, G. Mosca, P.Kersten, J. Wagner, Physik, Springer-Spektrum, Berlin, 2019.
- H. Yersin (Hrsg.): Highly Efficient OLEDs, Wiley-VCH, Weinheim, 2019.
- R. Mertens, The OLED Handbook, A Guide to OLED Technology, Industry & Market, Metalgrass, Kfar Saba, Isreal, 2020.

R&D Project Management in the Chemical Industry

Supplementary Module 03 for Chemists (m/f/d)

Information Material *for the subject matter:*
Clear Coats for Automobiles, ***Chemistry and Physics****.*

Solvent Reduced Clear Coat for the Automotive Production.

Rainer Buerstinghaus

R&D Project Management in the Chemical Industry

Subject Matter	***Chemistry and Physics***

Solvent Reduced Clear Coat for the Automotive Production.

Solvent Reduced Clear Coat for the Automotive Production

Background (Legislation; Social Demands):

Climate protection demands (since 1990)

Reduction of the emissions of organic solvents in automobile production by 2/3.

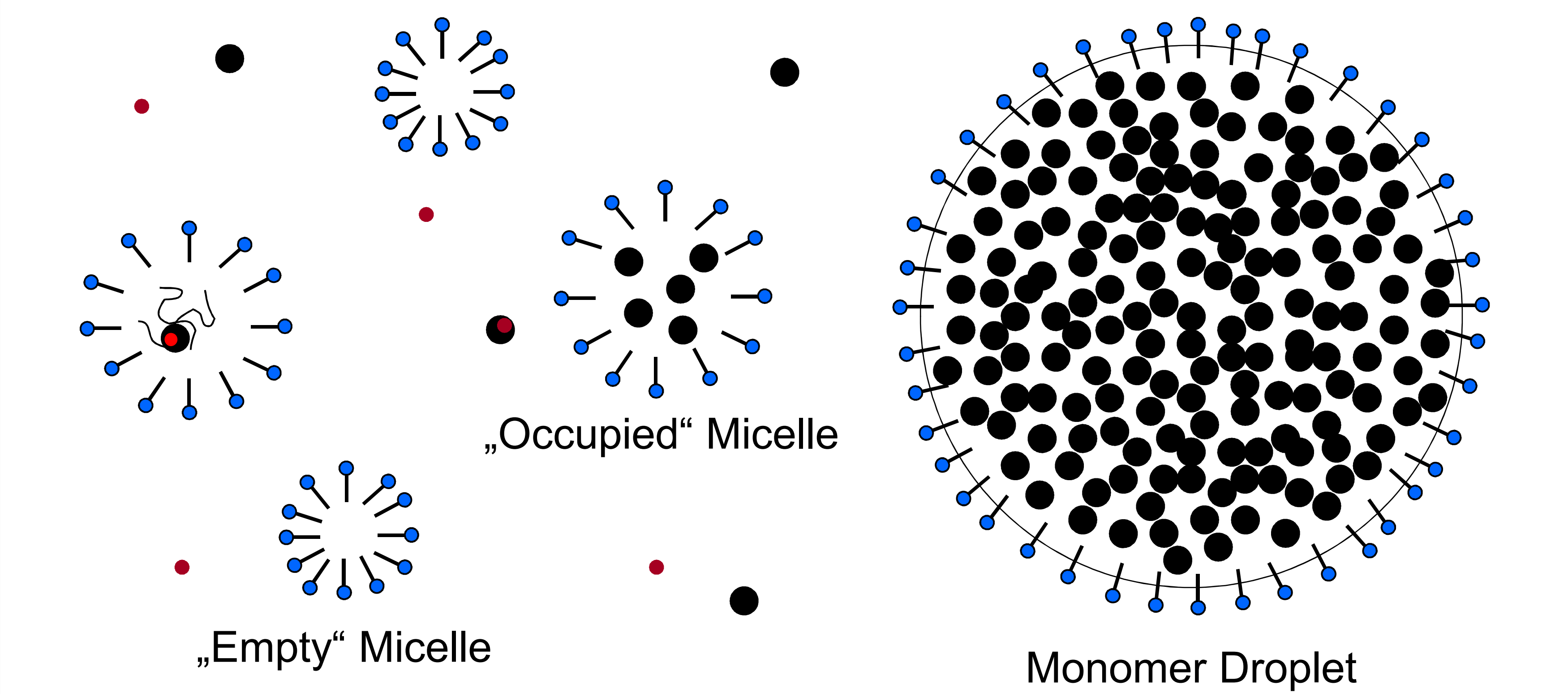
The **cosolvent content in the liquid lacquer must not exceed 20%** by weight (compared to 60% by weight in conventional lacquers).

VOC 130-140 g/l. (VOC: Volatile Organic Compounds)

$$\text{VOC (g/l)} = \frac{\text{mass of volatile components (g)} - \text{mass of water (g)}}{\text{volume of paint (l)} - \text{volume of water (l)}}$$

Rainer Buerstinghaus

Emulsion Polymerization, Phase 1: Particle Formation.

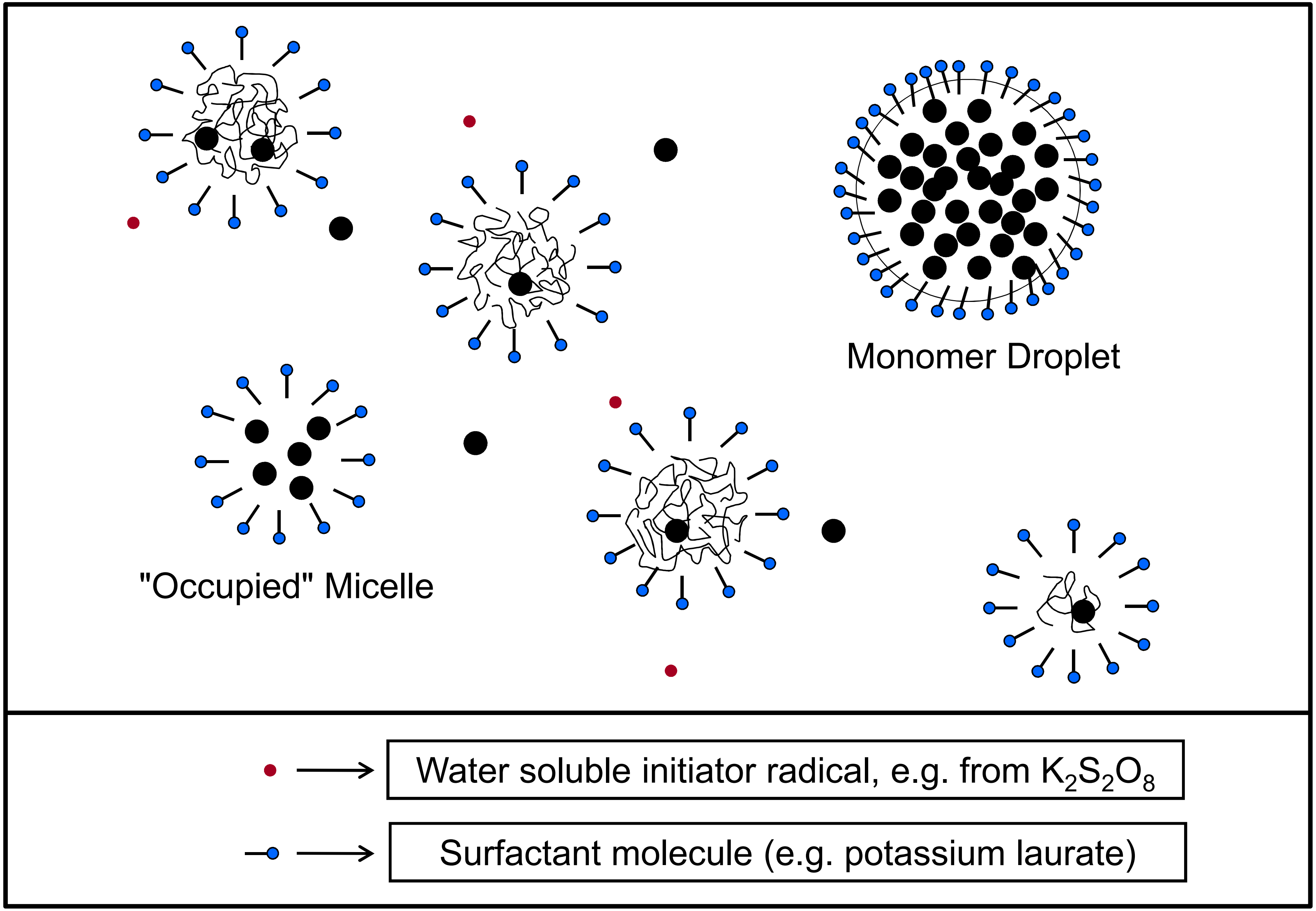


• ⟶ Water soluble initiator radical, e.g. from $K_2S_2O_8$:
$S_2O_8^{2-} + Fe^{2+} \longrightarrow SO_4^{2-} + SO_4^{\bullet -} + Fe^{3+}$

⟶ Surfactant molecule (e.g. potassium laurate)

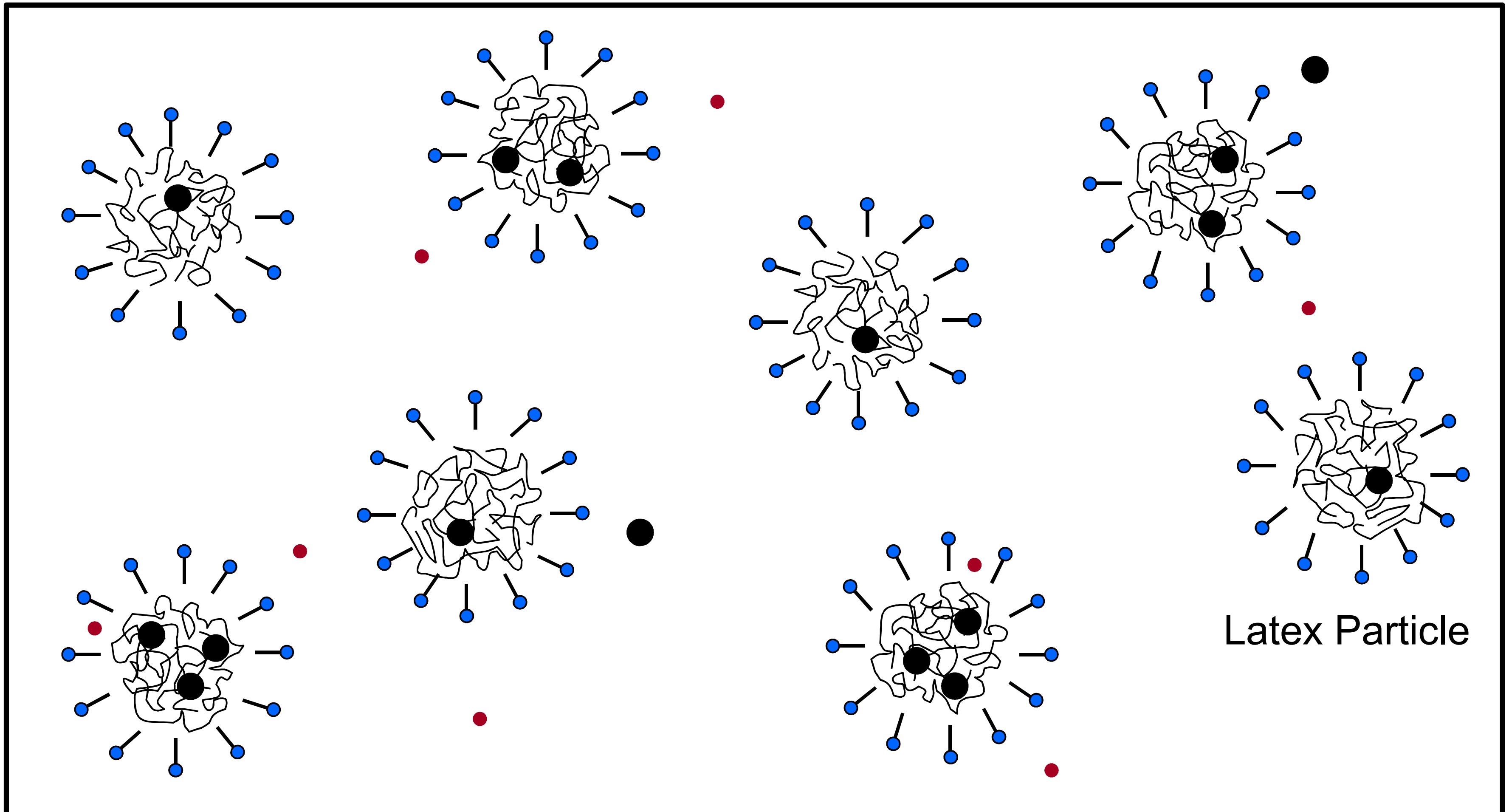
Rainer Buerstinghaus

Emulsion polymerization, Phase 2: Particle Growth.



Rainer Buerstinghaus

Emulsion Polymerization, Phase 3: Disappearance of Monomer.

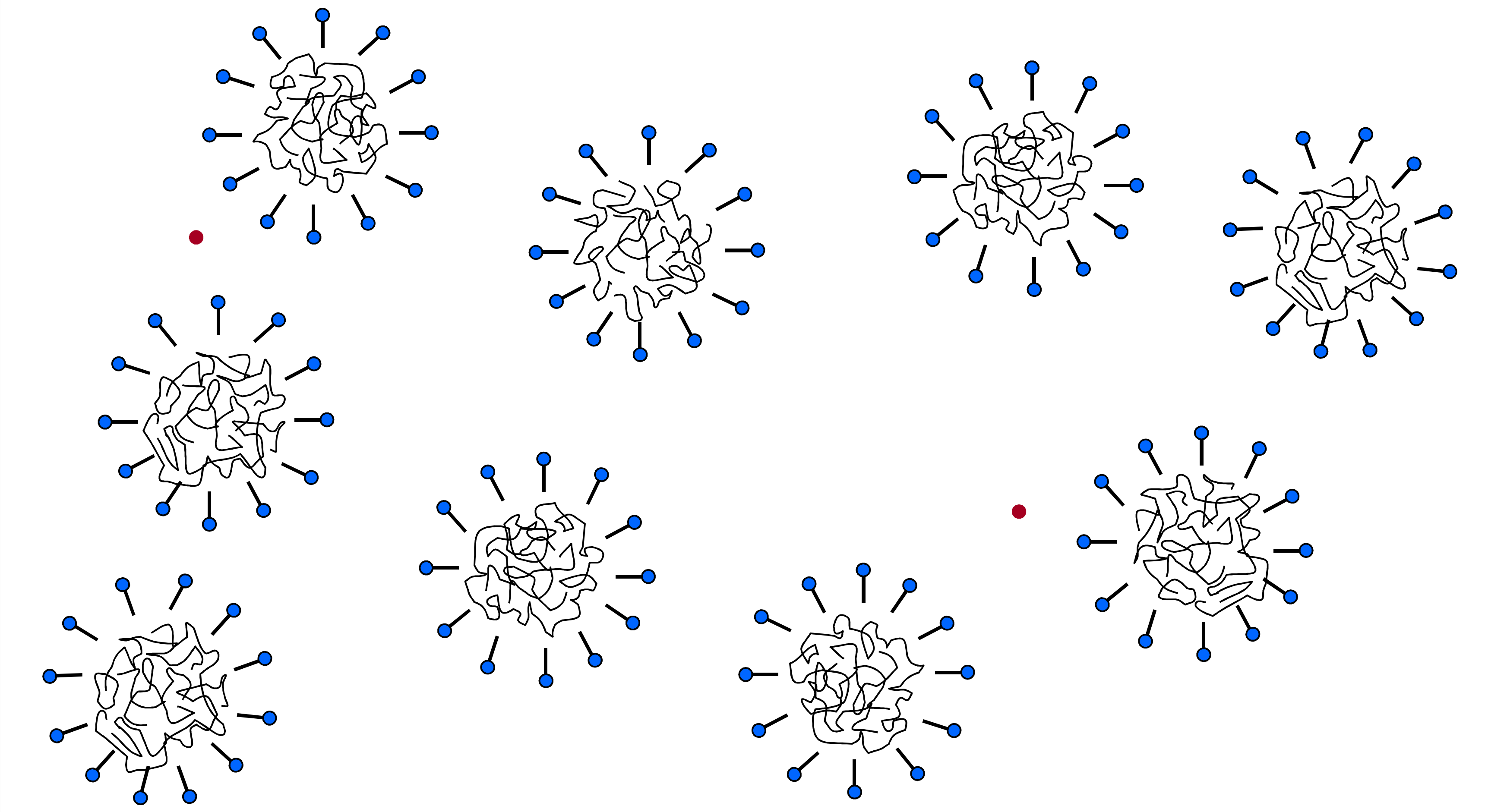


Water soluble initiator radical, e.g. from $K_2S_2O_8$

Primary dispersion; Particle−Ø: 1 – 100 nm

Rainer Buerstinghaus

Emulsion Polymerization, Phase 4: End of the Reaction.



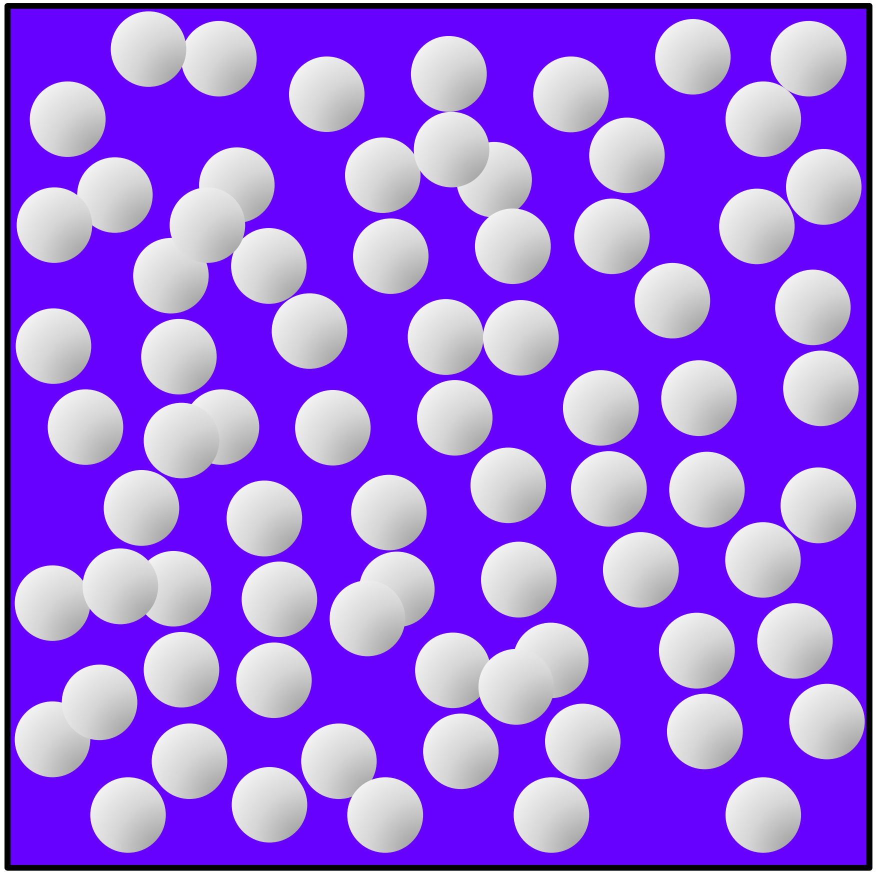
Water soluble initiator radical, e.g. from $K_2S_2O_8$

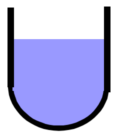
Primary dispersion; Particle−Ø: 1 – 100 nm

Rainer Buerstinghaus

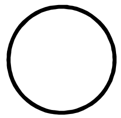
Solvent Reduced Clear Coat for the Automotive Production

Emulsion Polymer, Primary Dispersion, Monodisperse.

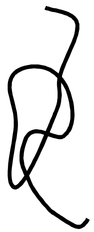




1 ml of primary dispersion contains ≈ 10^{15} Particles (1 Quadrillion).



One primary particle contains between 1 and 10.000 macromolecules.



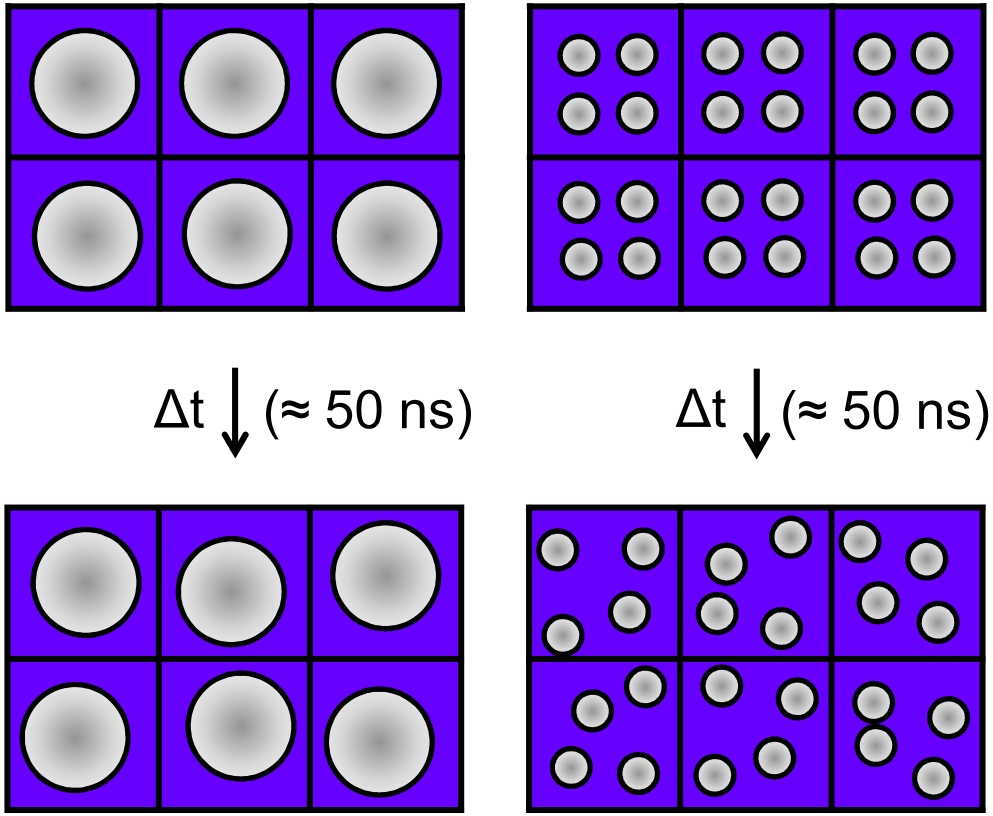
One macromolecule contains between 10^2 and 10^6 monomer units.

Rainer Buerstinghaus

Solvent Reduced Clear Coat for the Automotive Production

Dispersions: Particle Size Measurement, Basic Principle.

Initial distribution of the particles (idealized)



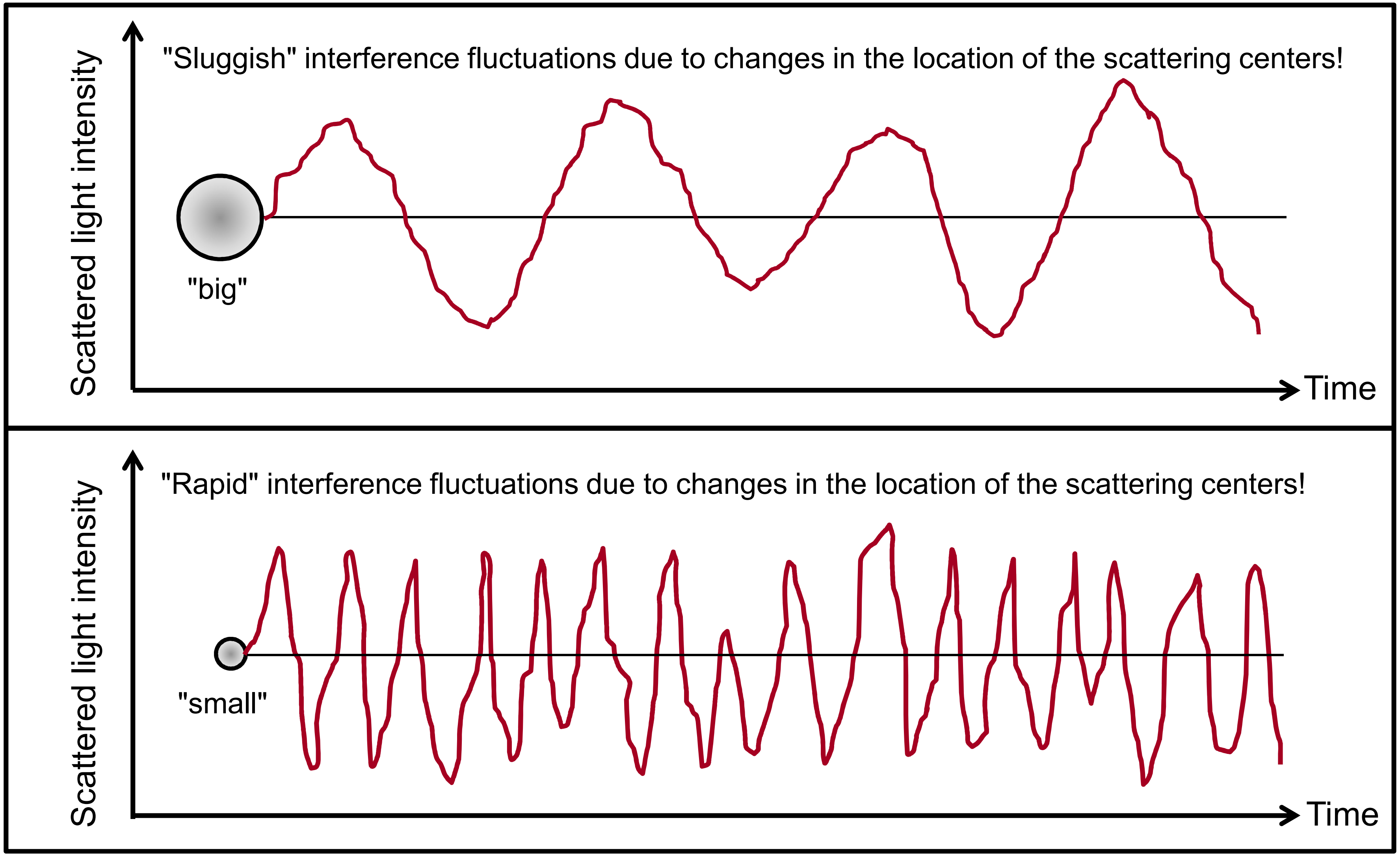
$$D = \frac{k_B\ T}{6\ \pi\ \eta\ R_0}$$

D	Diffusion Coefficient
k_B	Boltzmann Constant
T	Temperature (Kelvin)
η	Dynamic Viscosity of the Liquid Phase.
R_0	Hydrodynamic Radius of the Particles.

Stokes-Einstein Equation:
The particle radius is inversely proportional to the diffusion coefficient.

Solvent Reduced Clear Coat for the Automotive Production

Dispersions: Particle Size Measurement, Basic Principle.

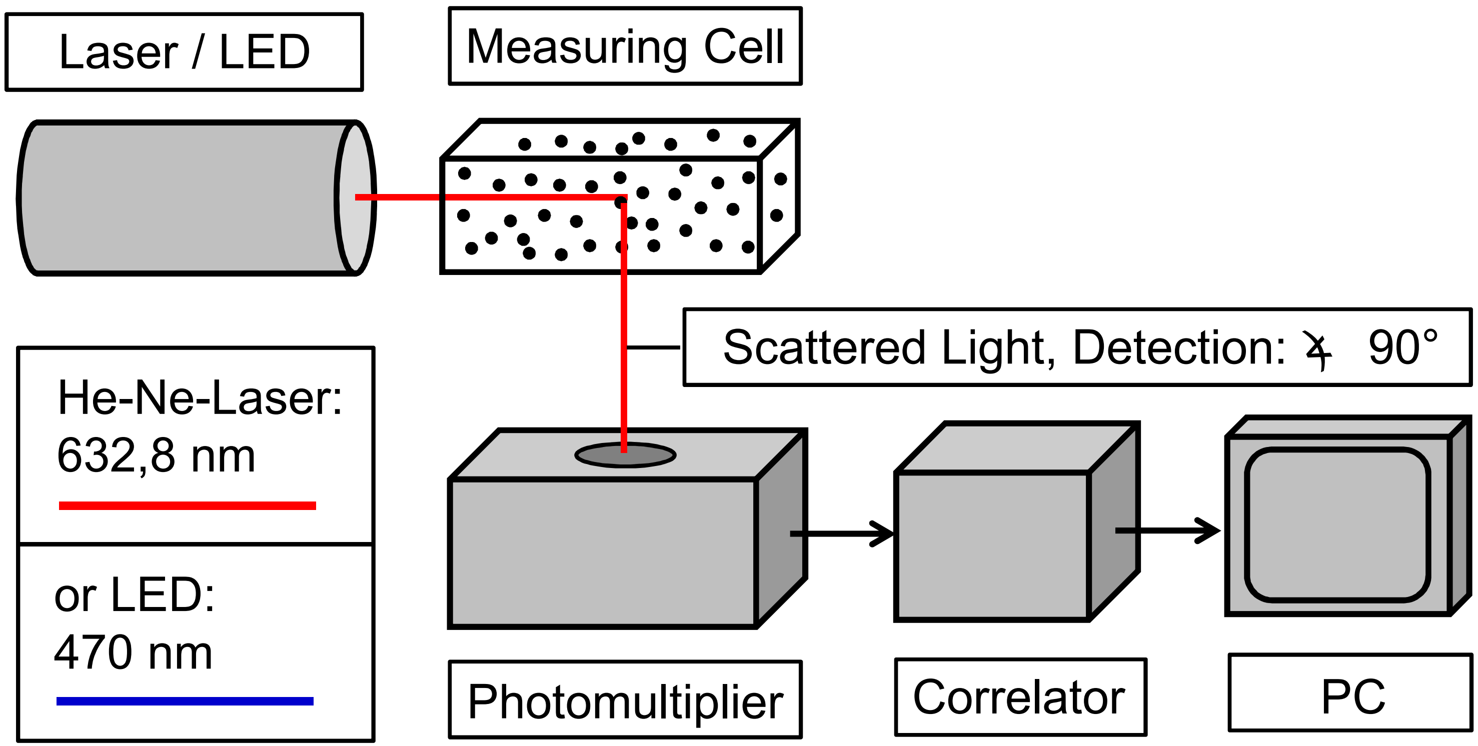


Rainer Buerstinghaus

Solvent Reduced Clear Coat for the Automotive Production

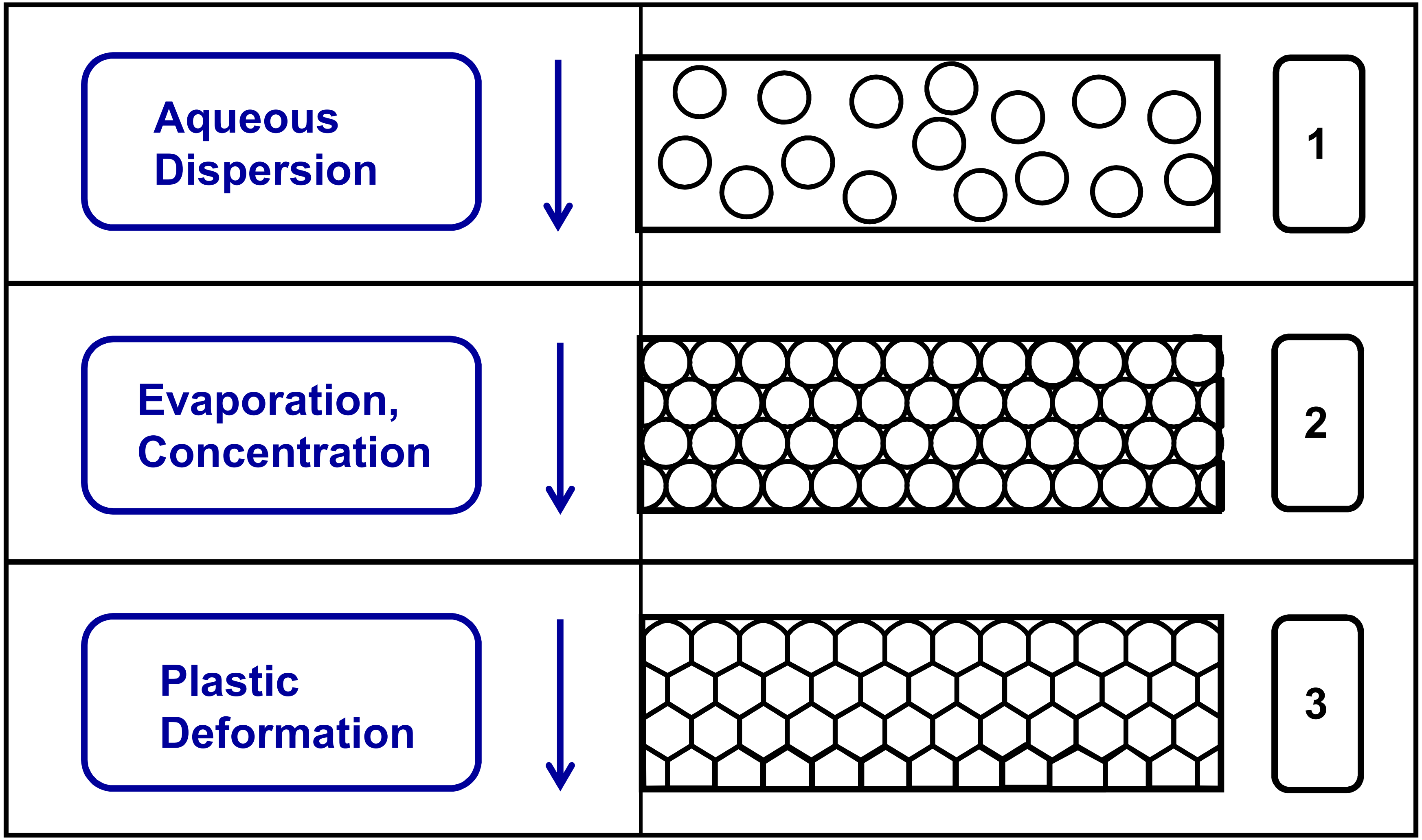
Dispersions: Particle Size Measurement, Basic Principle.

Construction principle of a device for measuring particle diameters by means of quasi-elastic, dynamic light scattering.



Solvent Reduced Clear Coat for the Automotive Production

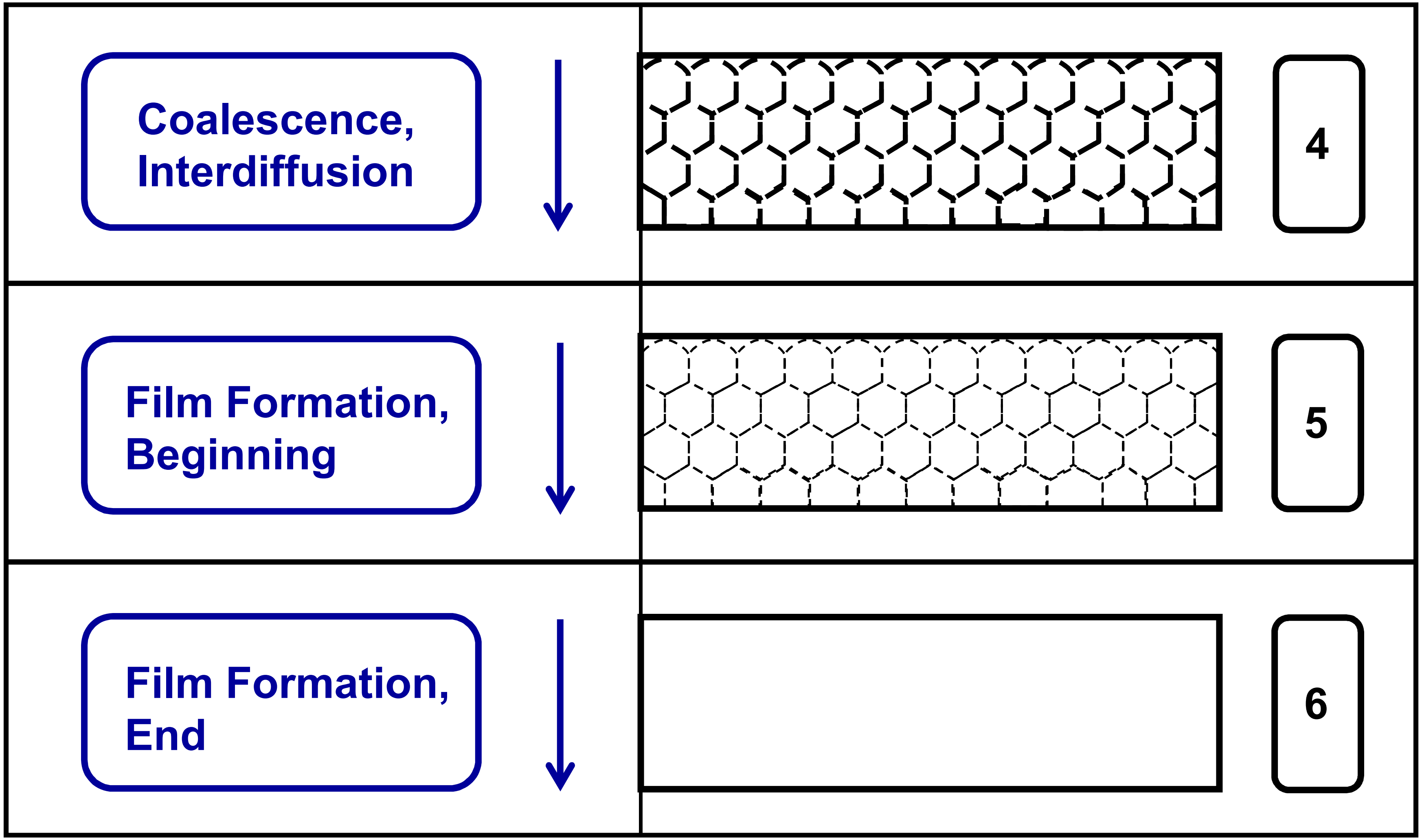
Emulsion Polymer, Film Formation Mechanism.



Rainer Buerstinghaus

Solvent Reduced Clear Coat for the Automotive Production

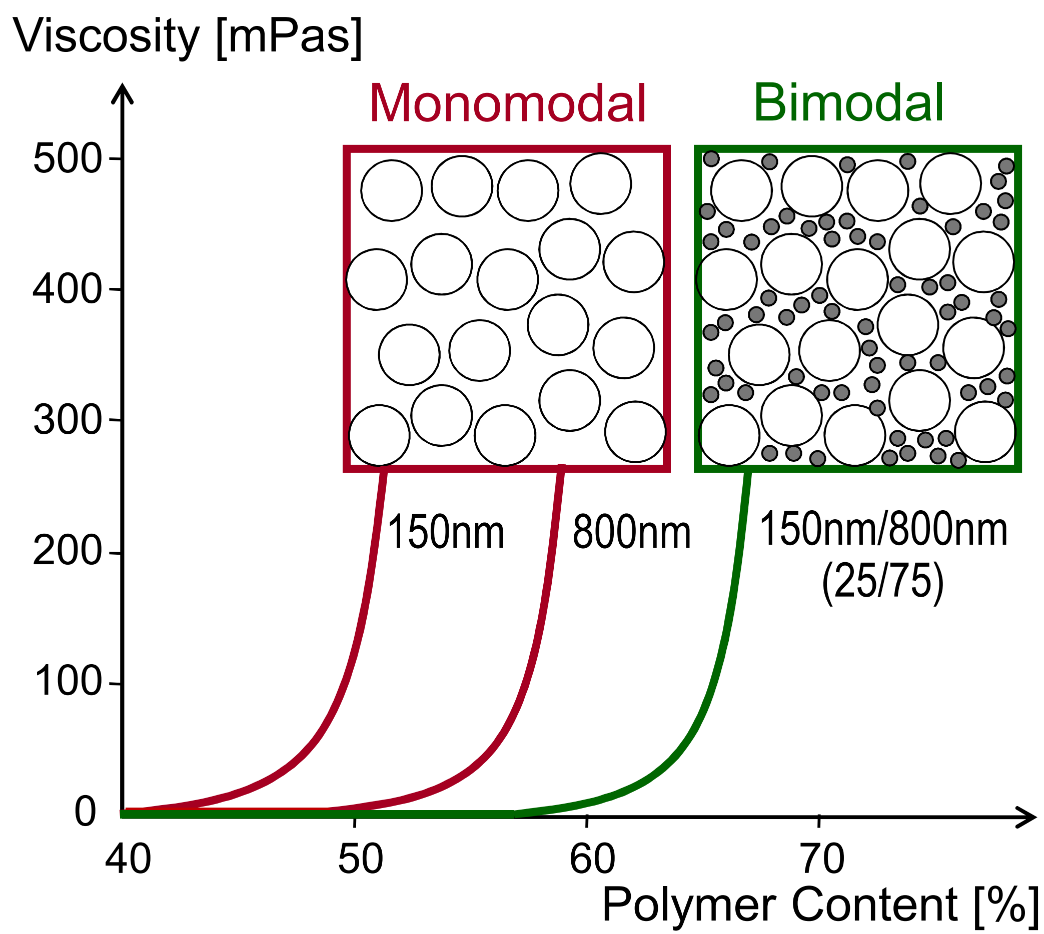
Emulsion Polymer, Film Formation Mechanism.



Rainer Buerstinghaus

Solvent Reduced Clear Coat for the Automotive Production

Emulsion Polymer, Primary Dispersion; Viscosity as a Function of Solids Content.



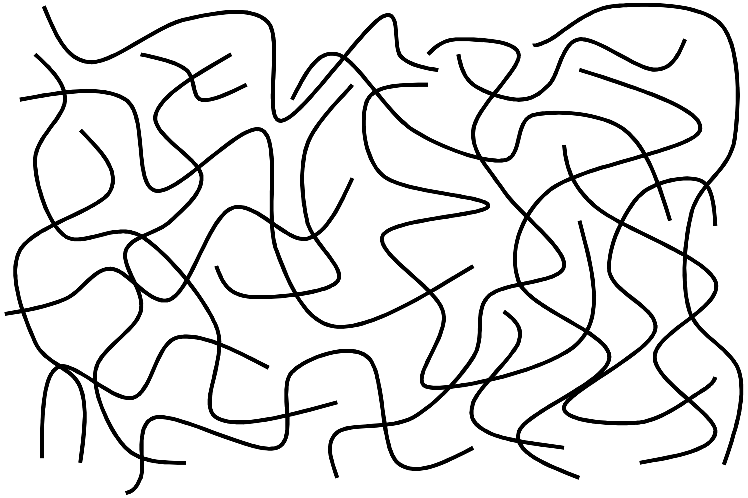
The viscosity as a function of the polymer content depends strongly on the particle size and on the particle size distribution.

Rainer Buerstinghaus

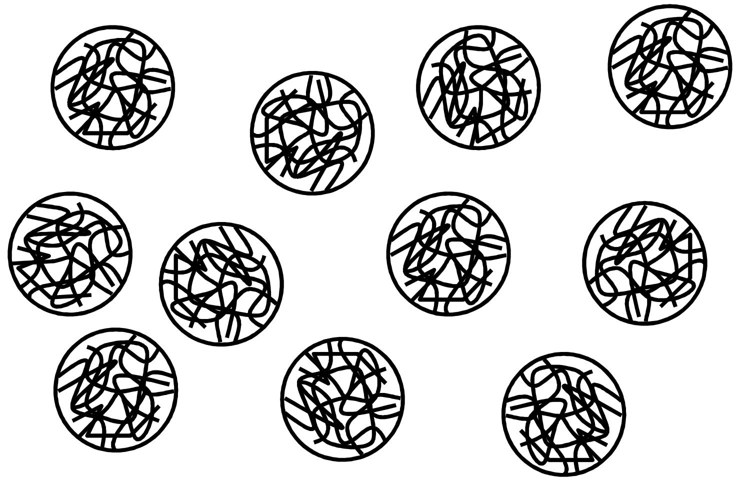
Solvent Reduced Clear Coat for the Automotive Production

Solutions/Dispersions: Viscosity and Molecular Weight.

Polymer Solution



Polymer Dispersion



Viscosity

- Dependent of the molecular weight.
- Dependent of the concentration.

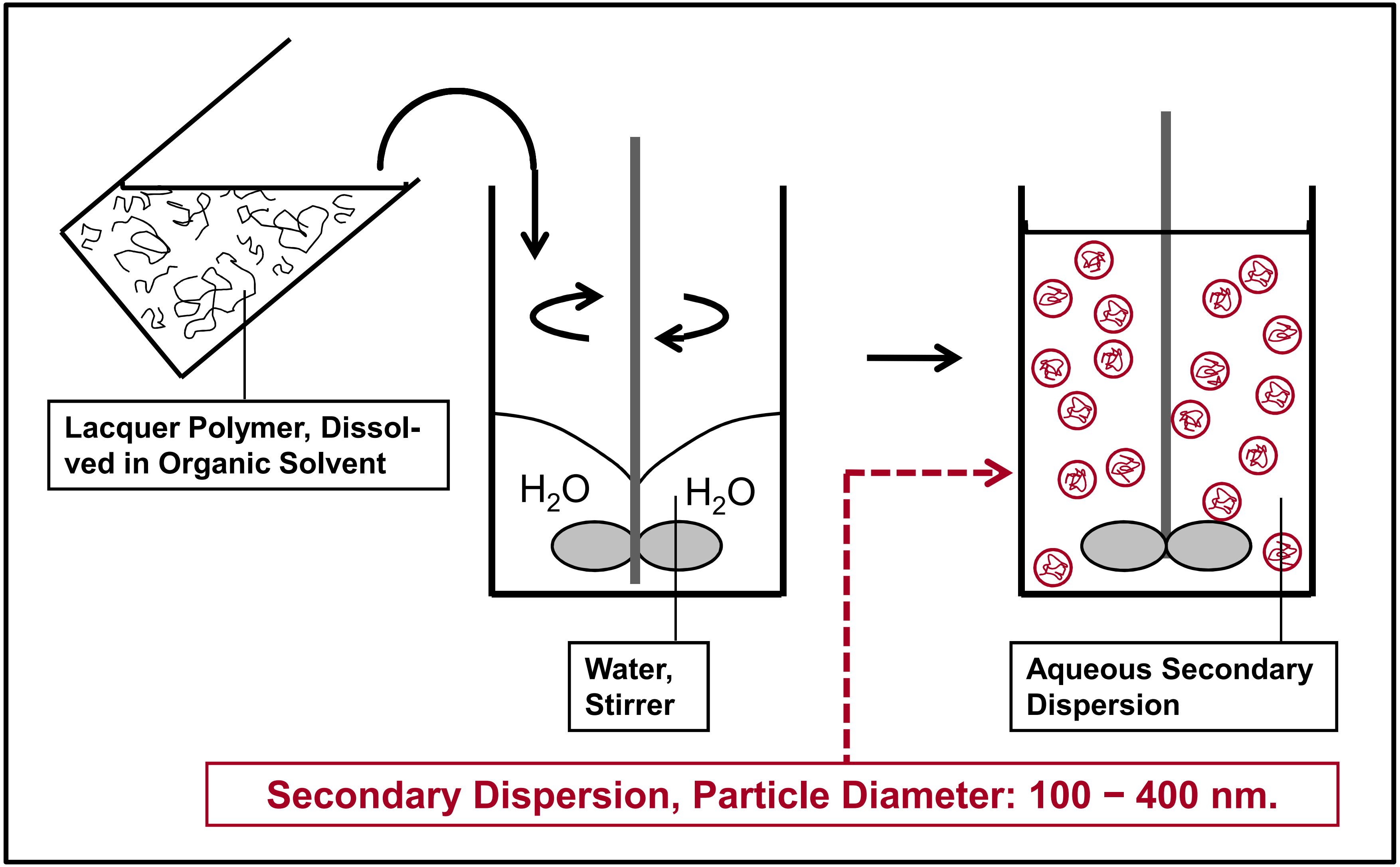
Viscosity

- **Independent** of the molecular weight.
- **Dependent** of the concentration.

Rainer Buerstinghaus

Solvent Reduced Clear Coat for the Automotive Production

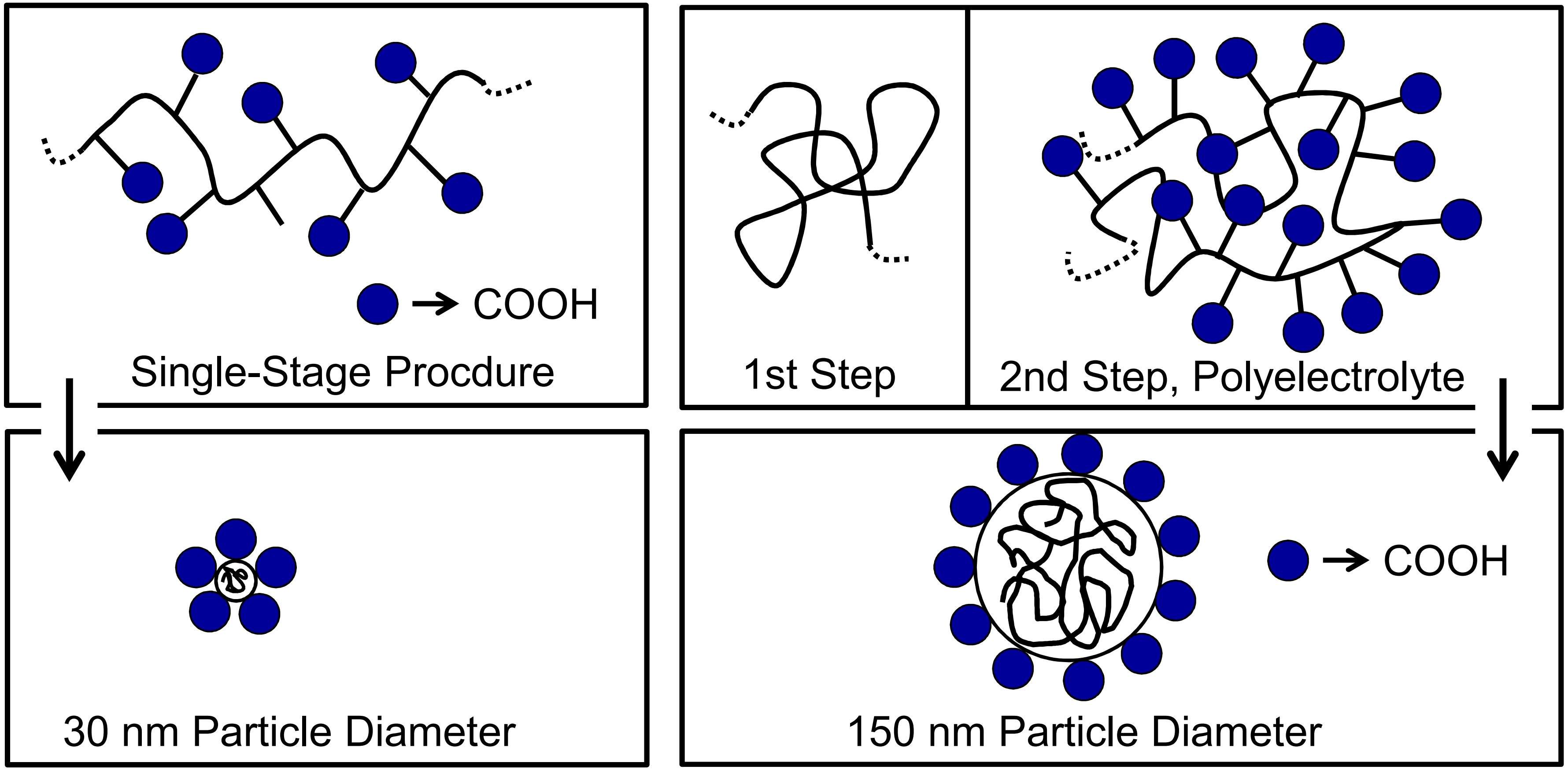
Generation of a Paint Resin Secondary Dispersion.



Rainer Buerstinghaus

Solvent Reduced Clear Coat for the Automotive Production

Aqueous Clearcoat, Solution Approach: Secondary Dispersion.



Resin: 36% by weight of a secondary polyacrylate dispersion, **2-stage procedure,**
Crosslinkers: Melamine resin, blocked isocyanate.

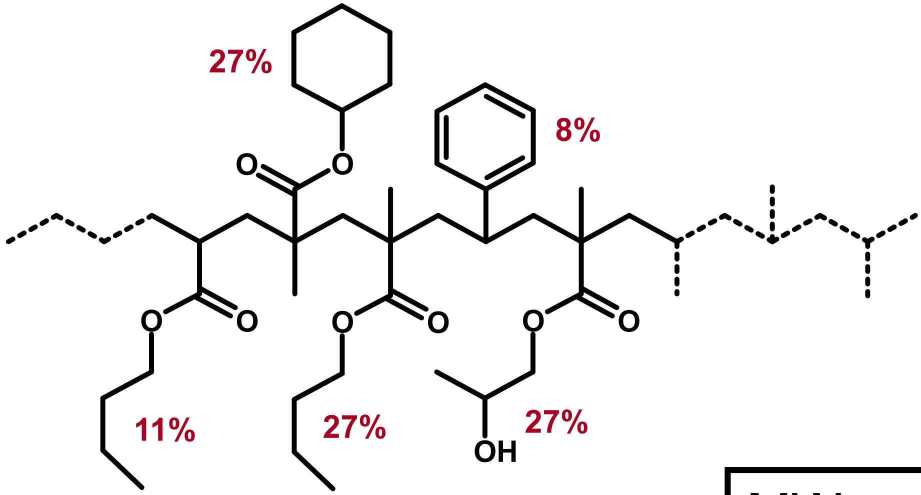
Co-Solvent: 16% by weight methoxypropanol, butyl diglycol and butanol
Dispersing medium: 48% by weight deionized water.

Rainer Buerstinghaus

Solvent Reduced Clear Coat for the Automotive Production

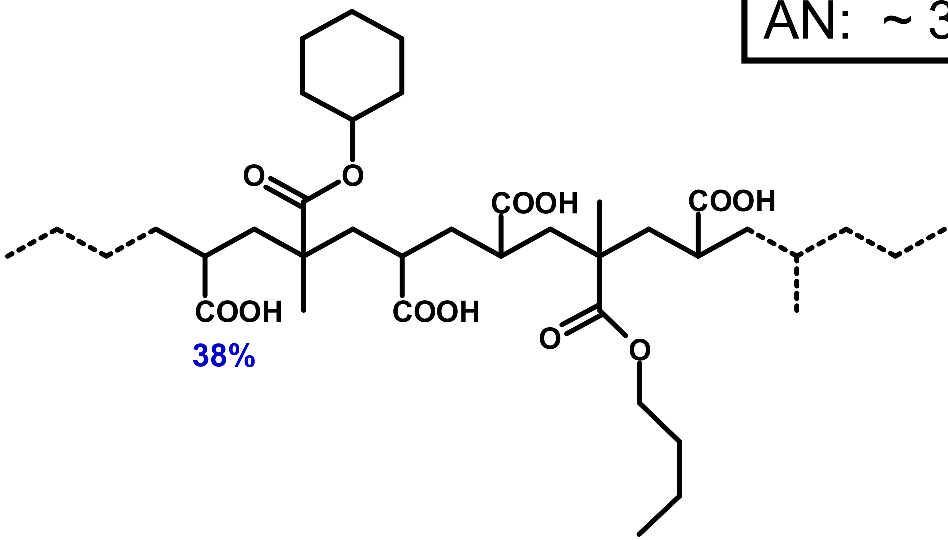
Aqueous Clear Coat: Secondary Acrylic Dispersion, Two-Stage.

Core:
Step 1



MW: ~ 8.500
AN: ~ 35

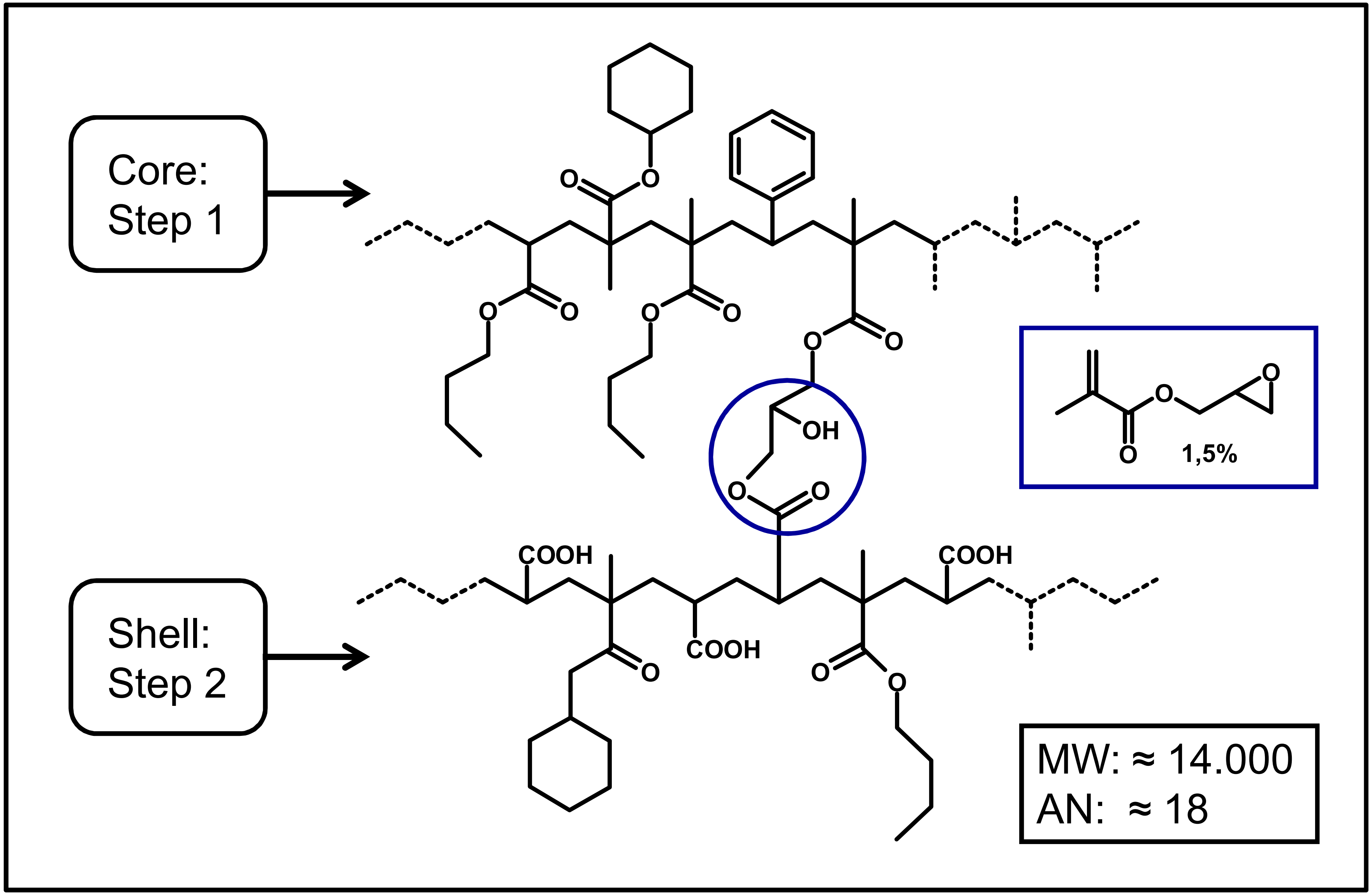
Shell:
Step 2



Rainer Buerstinghaus

Solvent Reduced Clear Coat for the Automotive Production

Aqueous Clear Coat: Sec. Acrylic Disp., Two-Stage, "Docked".



Further literature (specialist books, specialist articles) on the subject: "Solvent Reduced Clear Coat for the Automotive Production".

- D. Urban, K. Takamura, Polymer Dispersions and Their Industrial Applications, Wiley-VCH, Weinheim, 2002.
- H.-P. Rink in: H-J. Streitberger, K-F. Dössel, Automotive Paints and Coatings, Wiley-VCH, Weinheim, 2008, S. 211 ff.
- M. Brahm, Polymerchemie kompakt, Hirzel, Stuttgart, Leipzig, 2016.
- Kittel, Lehrbuch der Lacke und Beschichtungen, Band 2: W. Krauß: Bindemittel für lösemittelhaltige und lösemittelfreie Systeme, Hirzel, Stuttgart, Leipzig, 1998.
- A. Goldschmidt, H-J. Streitberger, BASF Handbuch Lackiertechnik, Vincentz, Hannover, 2014.
- S. Koltzenburg, M. Maskos, O. Nuyken, Polymere, Springer Spektrum, Heidelberg, 2014.
- B. Tieke, Makromolekulare Chemie, Wiley-VCH, Weinheim, 2014.
- M. D. Lechner, K. Gehrke, E. H. Nordmeier, Makromolekulare Chemie, Springer-Spektrum, Heidelberg, Berlin, 2014.
- C. Wrana, Polymerphysik, Springer-Spektrum, Heidelberg, Berlin, 2014.
- B. Müller, U. Poth, Lackformulierung und Lackrezeptur, Vincentz, Hannover, 2017.
- T. Brock, M. Groteklaes, P. Mischke, Lehrbuch der Lacktechnologie, Vincentz, Hannover, 2017.
- P. F. W. Simon, A. Fahmi, Polymere - Chemie und Strukturen, Wiley-VCH, Weinheim, 2020.

R&D Project Management
in the Chemical Industry

Supplementary Module 03 for Chemists (m/f/d)

Information Material *for the subject matter:*
Metal-Organic Frameworks, ***Further Areas of Use.***

Metal-Organic Frameworks,
Further Potential Areas of Application.

Rainer Buerstinghaus

New MOFs for the Adsorptive Storage of Gases

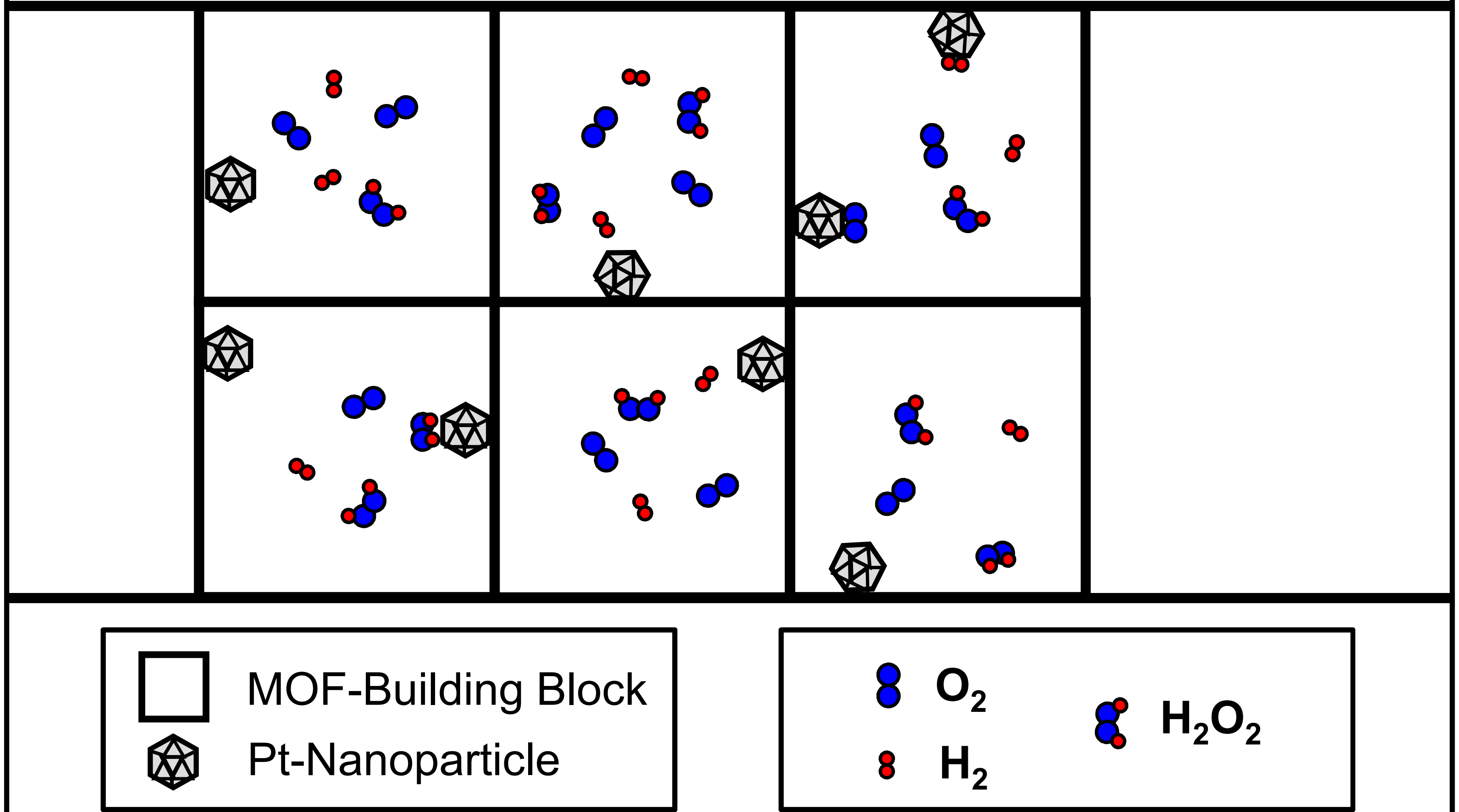
Technical Applications of these Porous Materials:

- Carrier materials for heterogeneous catalysis.
- Immobilization of (chiral) homogeneous catalysts.
- Nanoreactors.
- "Templates" on the nanoscale.
- Slow release formulations, controlled drug release.
- Luminescent lamps.
- Gas cleaning.
- Gas separation.
- Gas storage.

Metal-Organic Frameworks ⟶ Technical Applications

Carrier Materials for the Heterogeneous Catalysts:

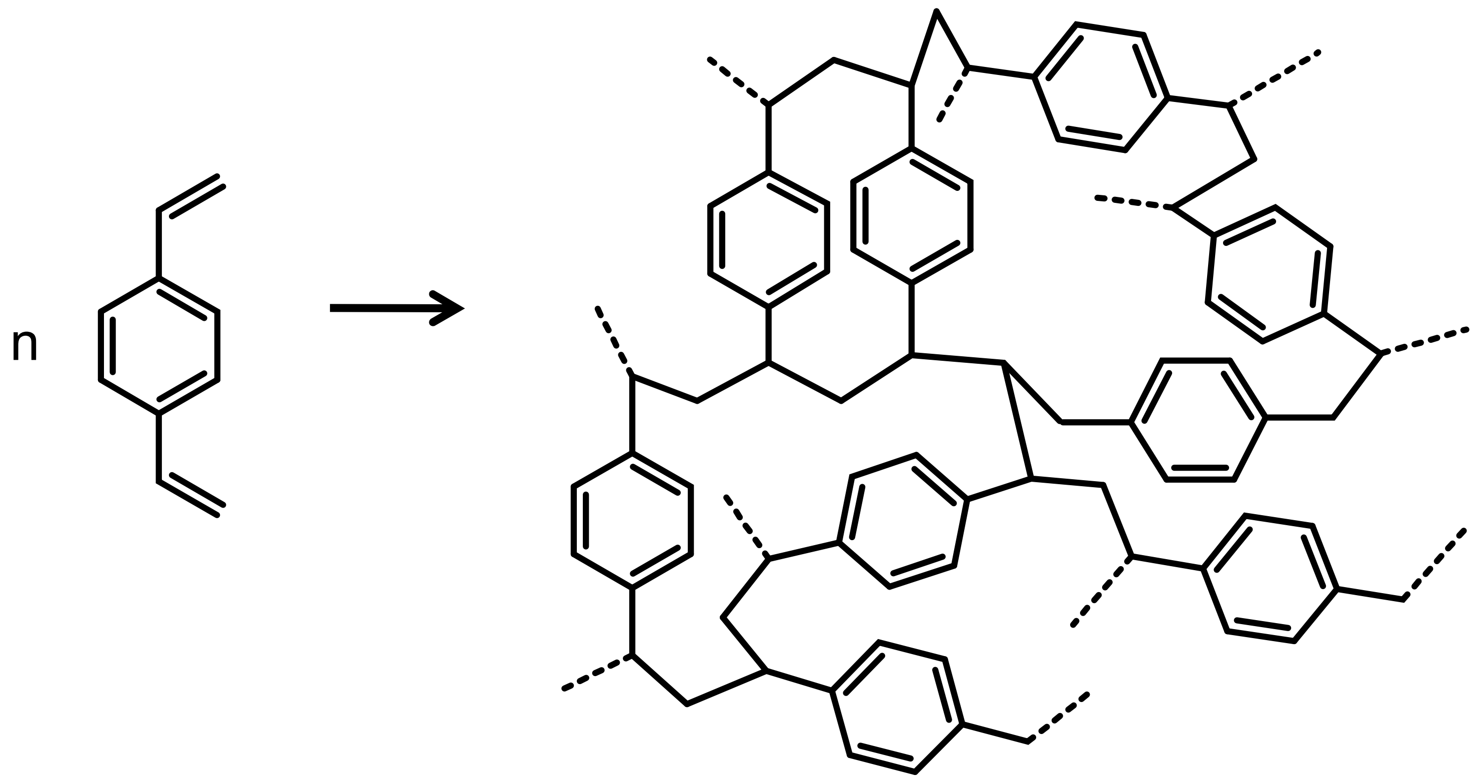
$$H_2 + O_2 \longrightarrow H_2O_2 \qquad (T < 100°C)$$



Rainer Buerstinghaus

Metal-Organic Frameworks ⟶ Technical Applications

Nanoreactor, Polymerization of DVB without "Shaping":

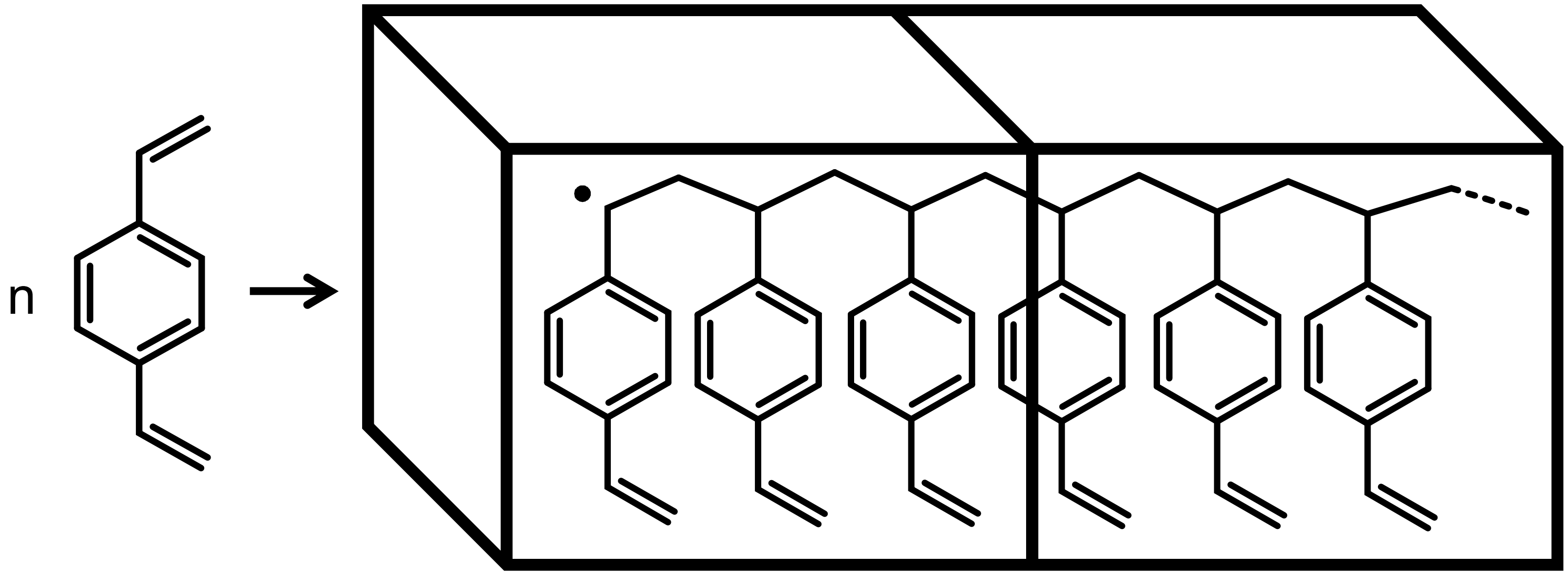


1,4- Divinylbenzene ⟶ Duromer, insoluble

Rainer Buerstinghaus

Metal-Organic Frameworks ⟶ Technical Applications

Nanoreactor, Topochemical Polymerization:



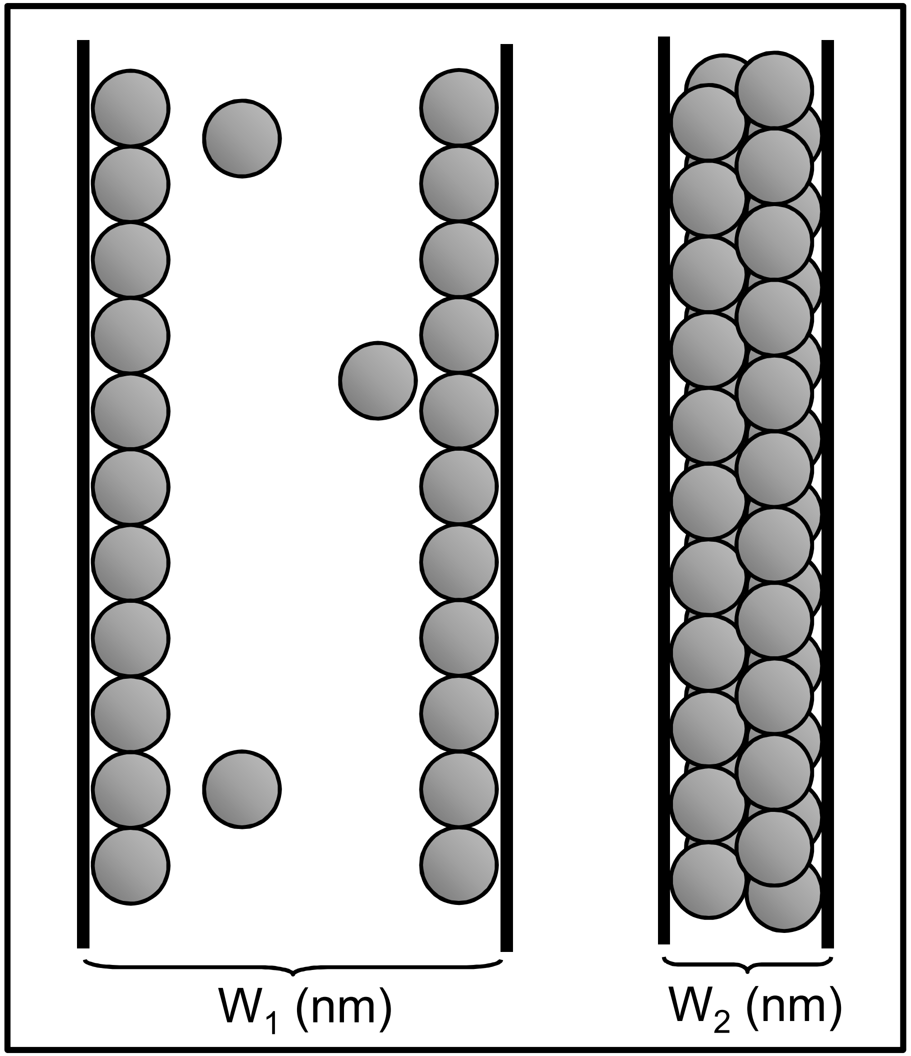
(100°C; 5 Days)

1,4- Divinylbenzene ⟶ Functionalized Polymer, soluble.

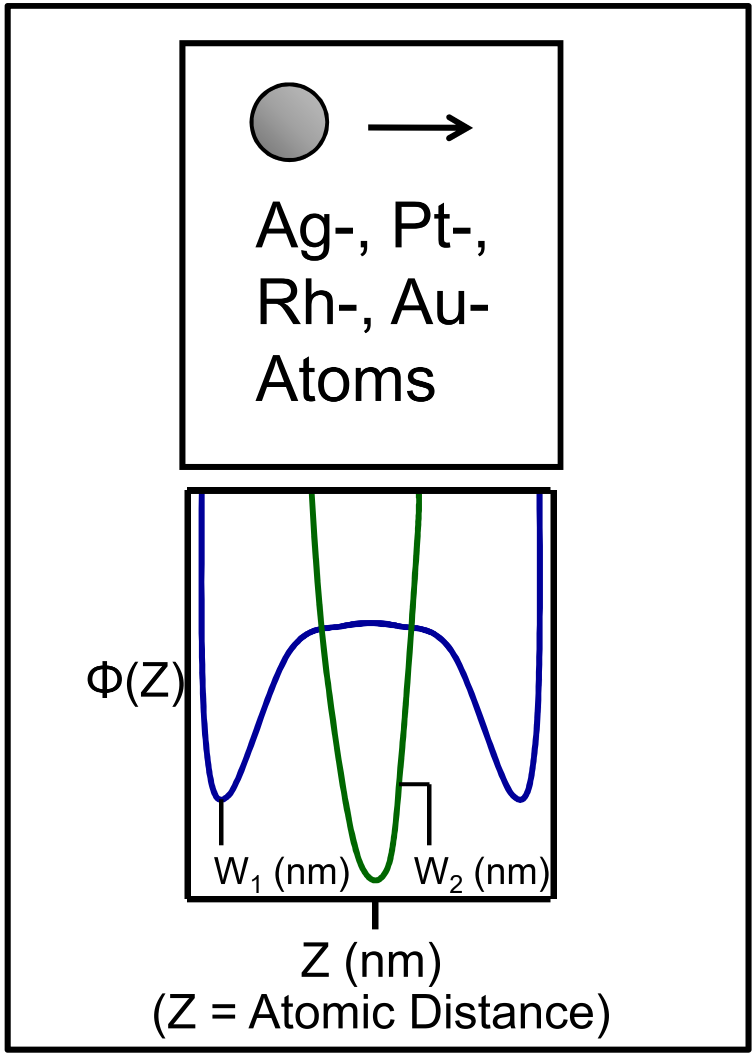
Rainer Buerstinghaus

Metal-Organic Frameworks → Technical Applications

Atomic / Molecular "Template" for Nano-Wires:



(W = Pore Width)

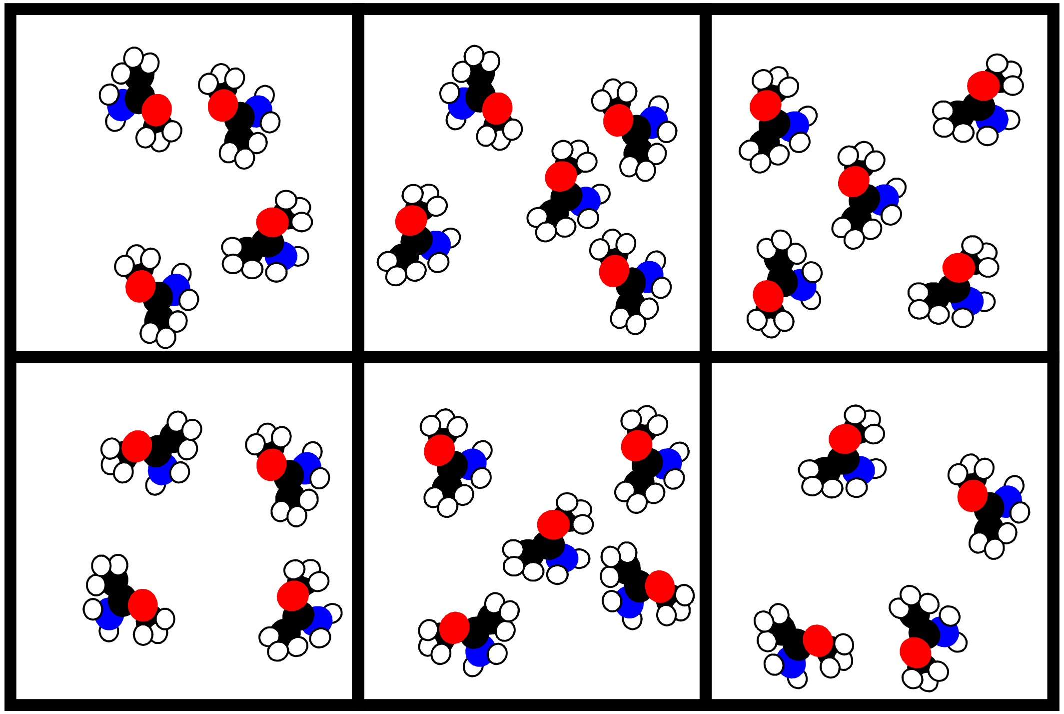


(Φ(Z) = Interaction Potential)

Rainer Buerstinghaus

Metal-Organic Frameworks ⟶ Technical Applications

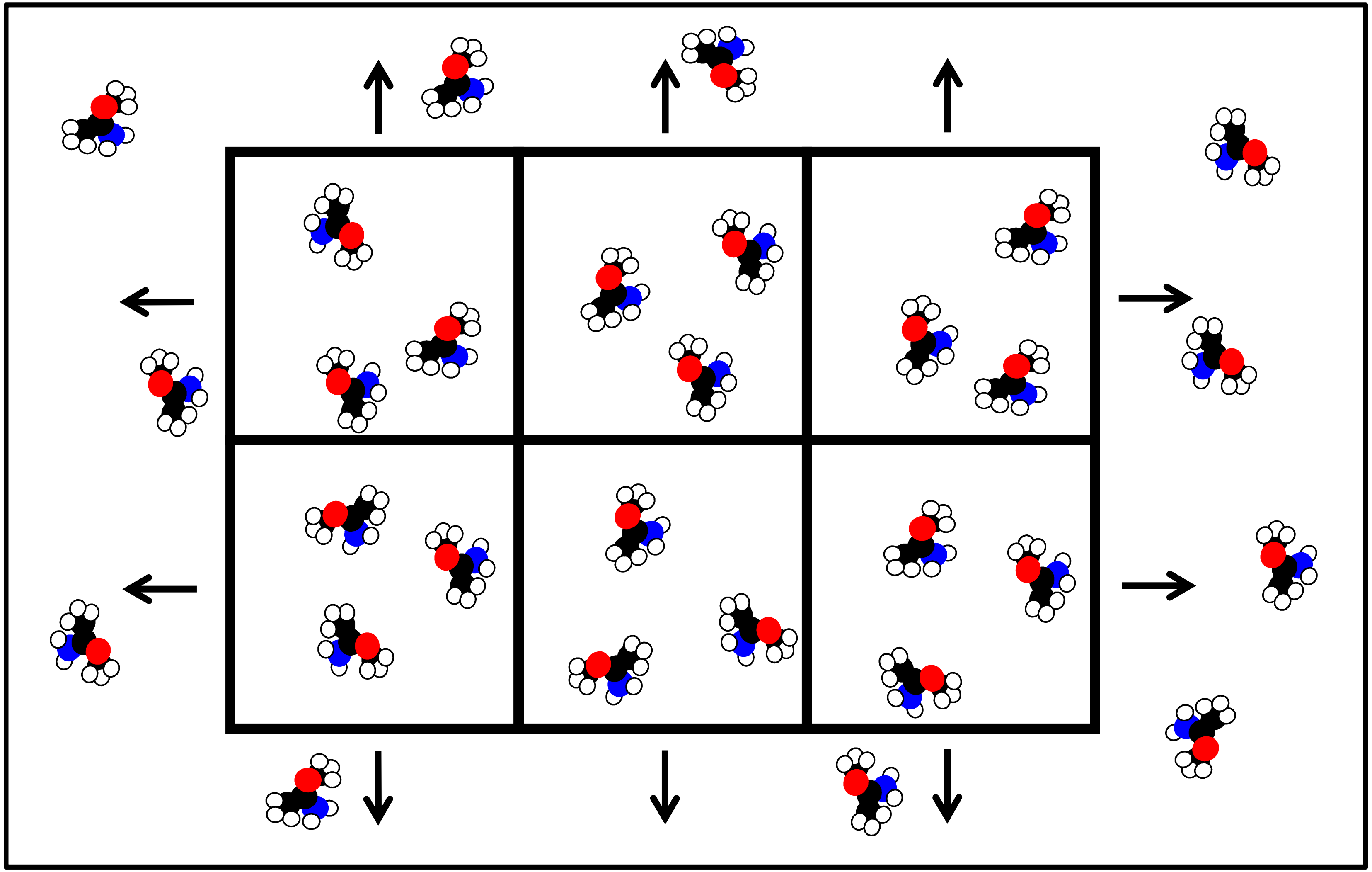
Slow Release, Controlled Release of Active Ingredients:



Rainer Buerstinghaus

Metal-Organic Frameworks ⟶ Technical Applications

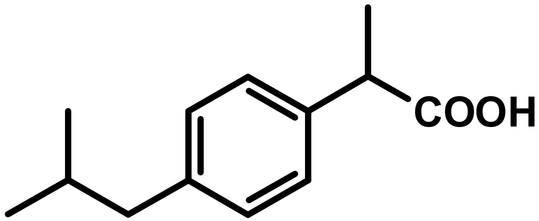
Slow Release, Controlled Release of Active Ingredients:



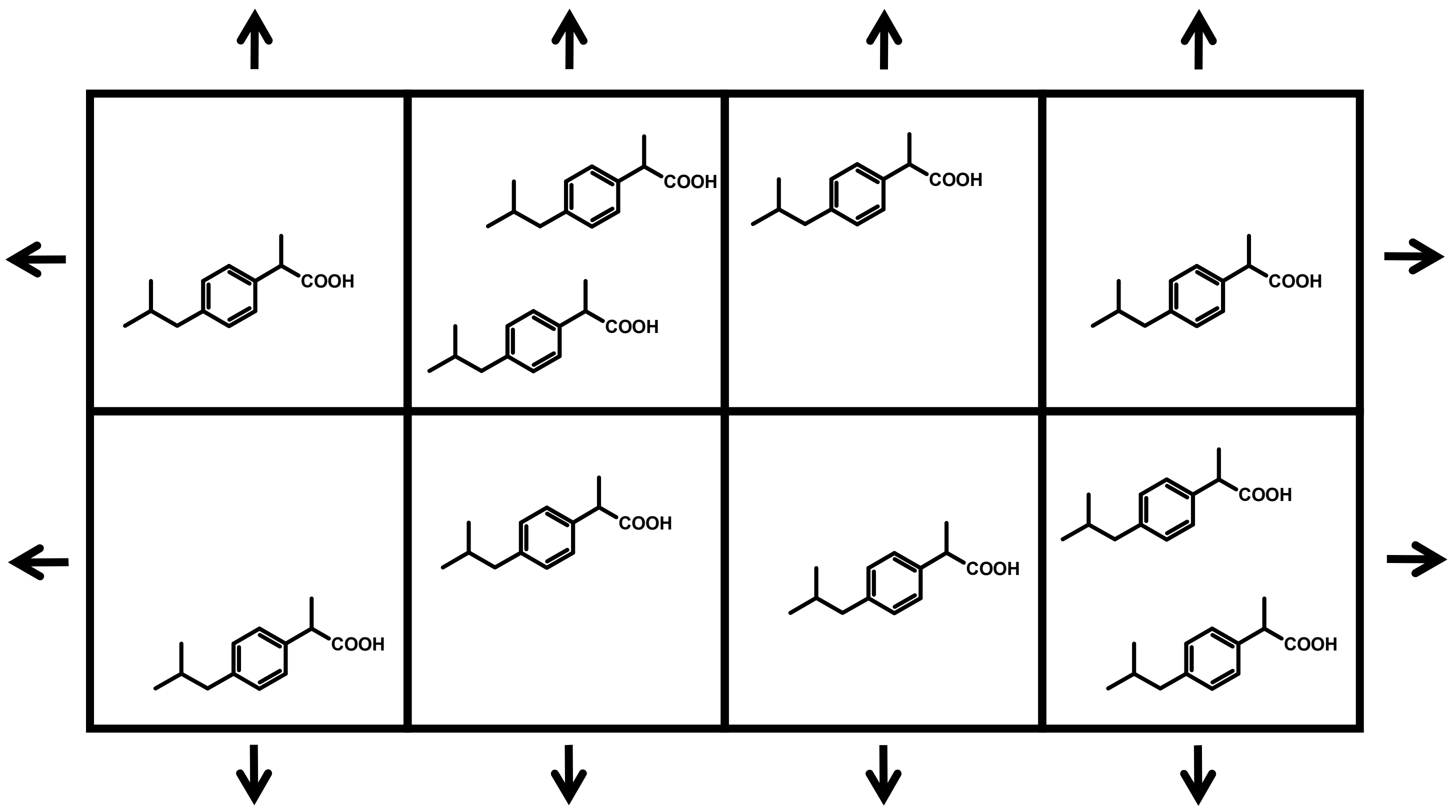
Rainer Buerstinghaus

Metal-Organic Frameworks ⟶ Technical Applications

Slow Release: Controlled Release of Ibuprofen® :

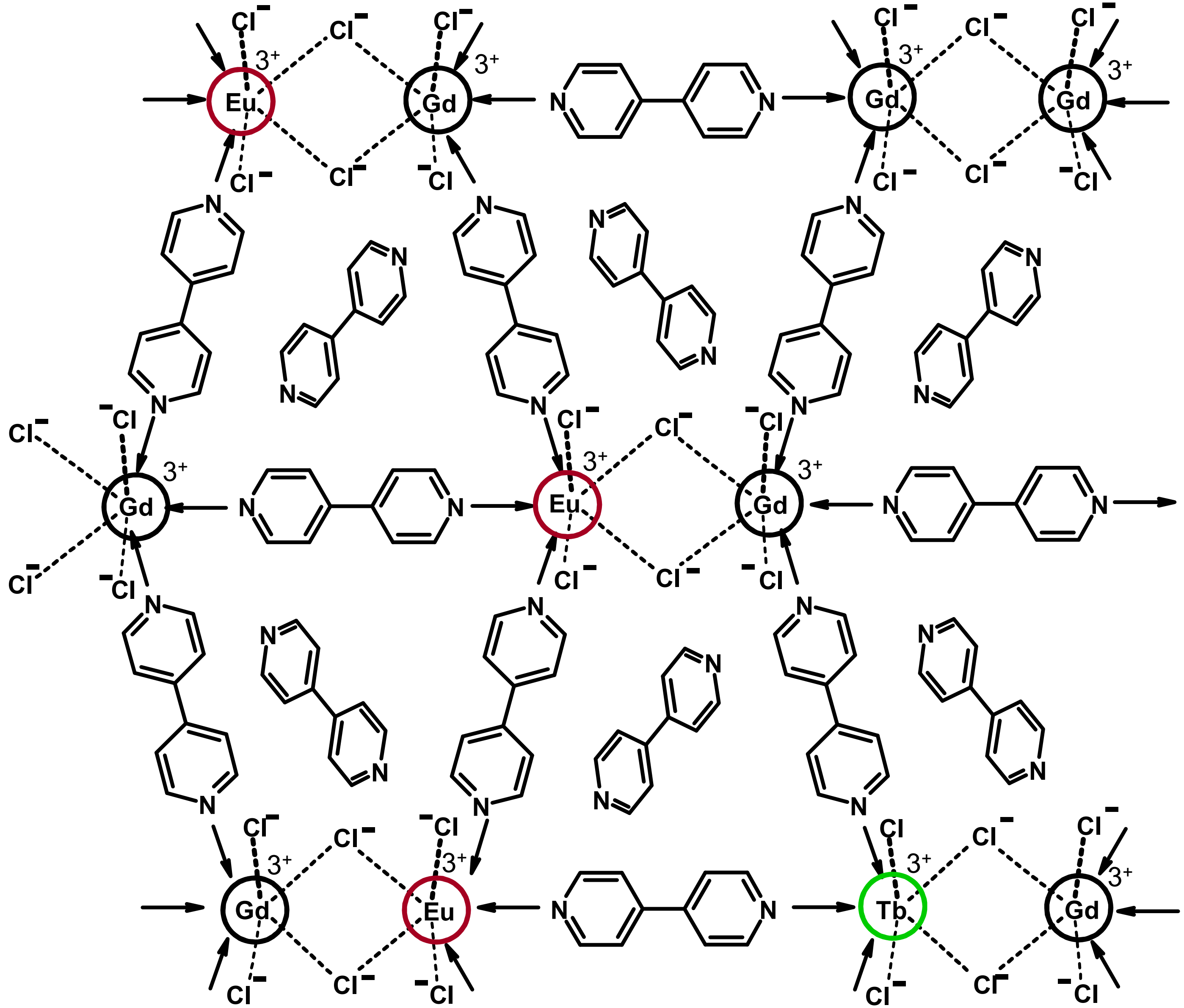


Ibuprofen® : Antirheumatic Drug
1,4g / g MOF-74: ⟶
Controlled release within 6 days.



Rainer Buerstinghaus

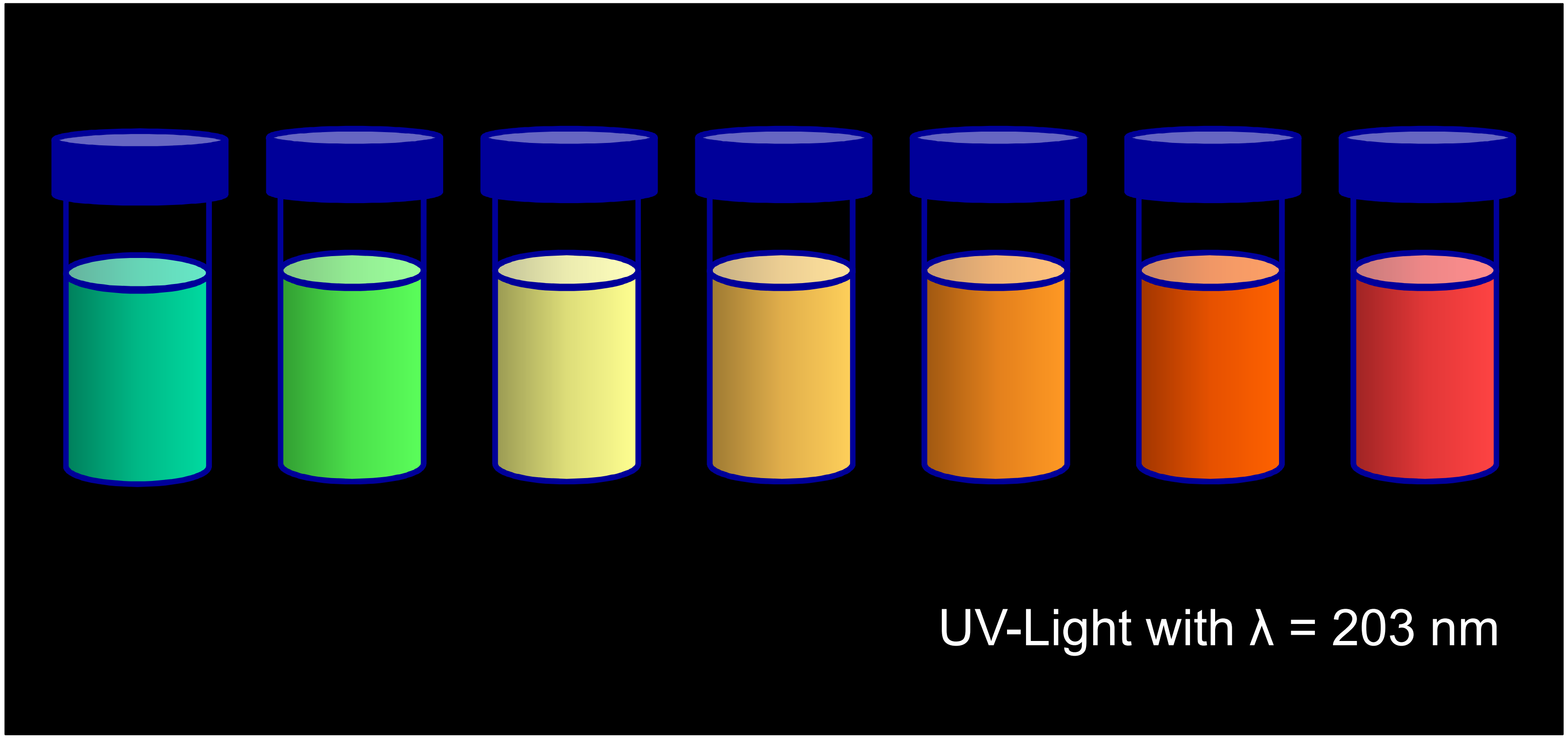
Metal-Organic Frameworks; Luminescence-Emitters with 4,4´-Bipyridyl as "Antennae" for UV-Light (302 nm):



Rainer Buerstinghaus

Metal-Organic Frameworks ⟶ Technical Applications

MOF-Luminescence Emitters with varying Gd-, Tb-, Eu- Ratios at λ = 203 nm. (Nachrichten aus der Chemie, 3/2013, S. 259)



Source: P.R. Matthes, C.J. Höller, M. Mai, J.Heck, S.J. Sedlmaier, S. Schmiechen, C. Feldmann, W. Schnick, K. Müller-Buschbaum, J. Mater. Chem. 2012, 22, 10179-10187

R&D Project Management in the Chemical Industry

Supplementary Module 03 for Chemists (m/f/d)

Information Material *for the subject matter:*
Ionic Liquids, ***Syntheses and Further Applications****.*

Ionic Liquids, Syntheses and Further Applications.

Rainer Buerstinghaus

R&D Project Management in the Chemical Industry

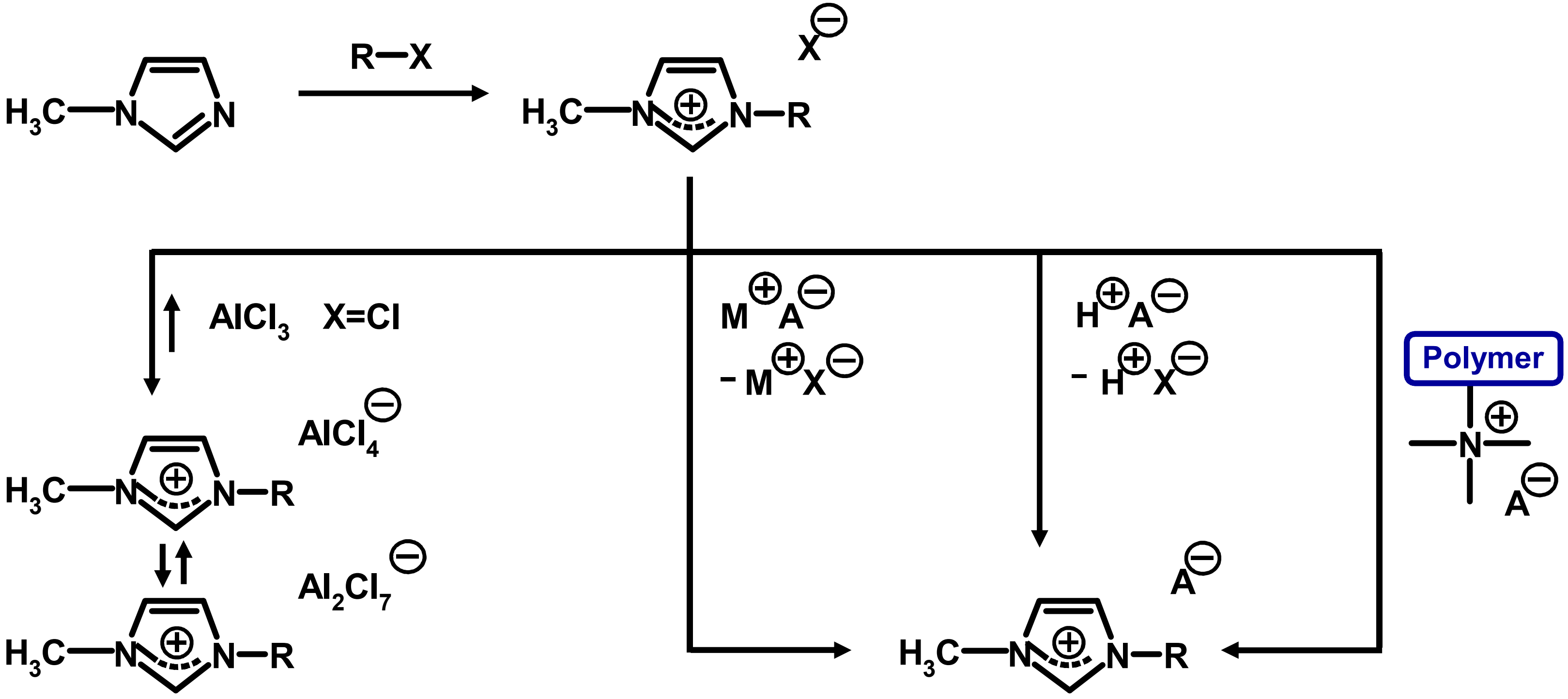
Subject Matter

Chemistry and Physics

Ionic Liquids,
Syntheses and Further Applications.

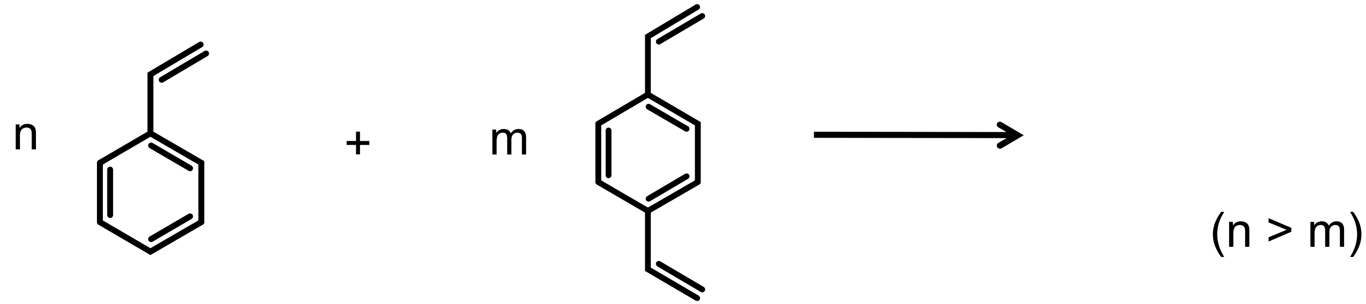
Rainer Buerstinghaus

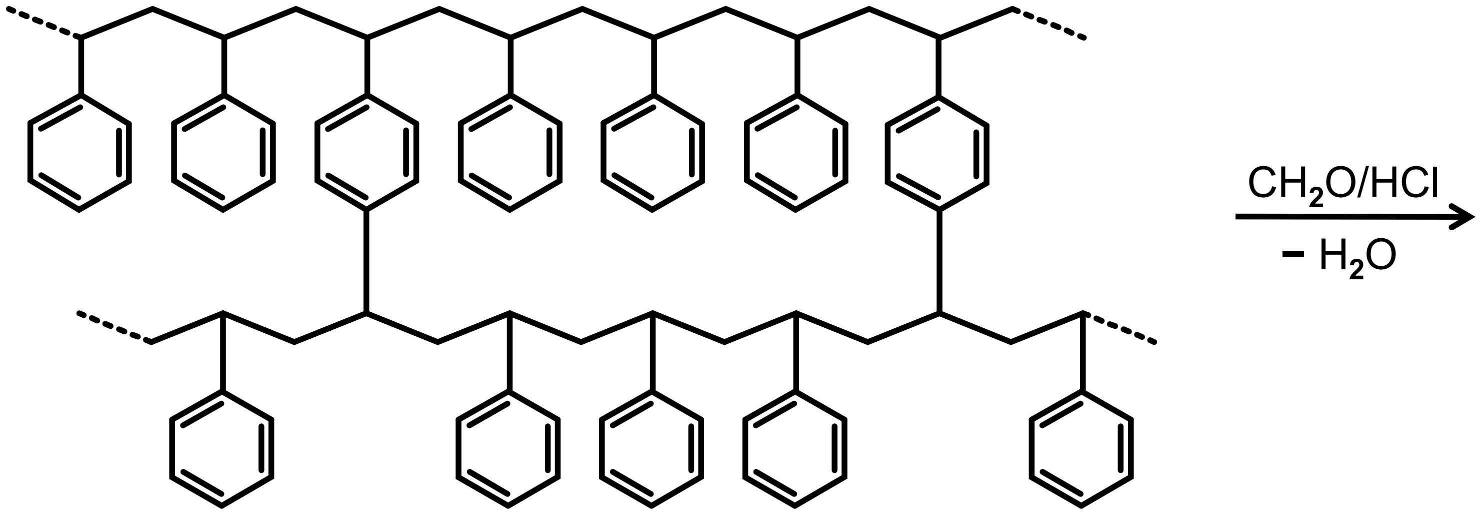
Ionic Liquids: Typical (Technical) Synthetic Routes.



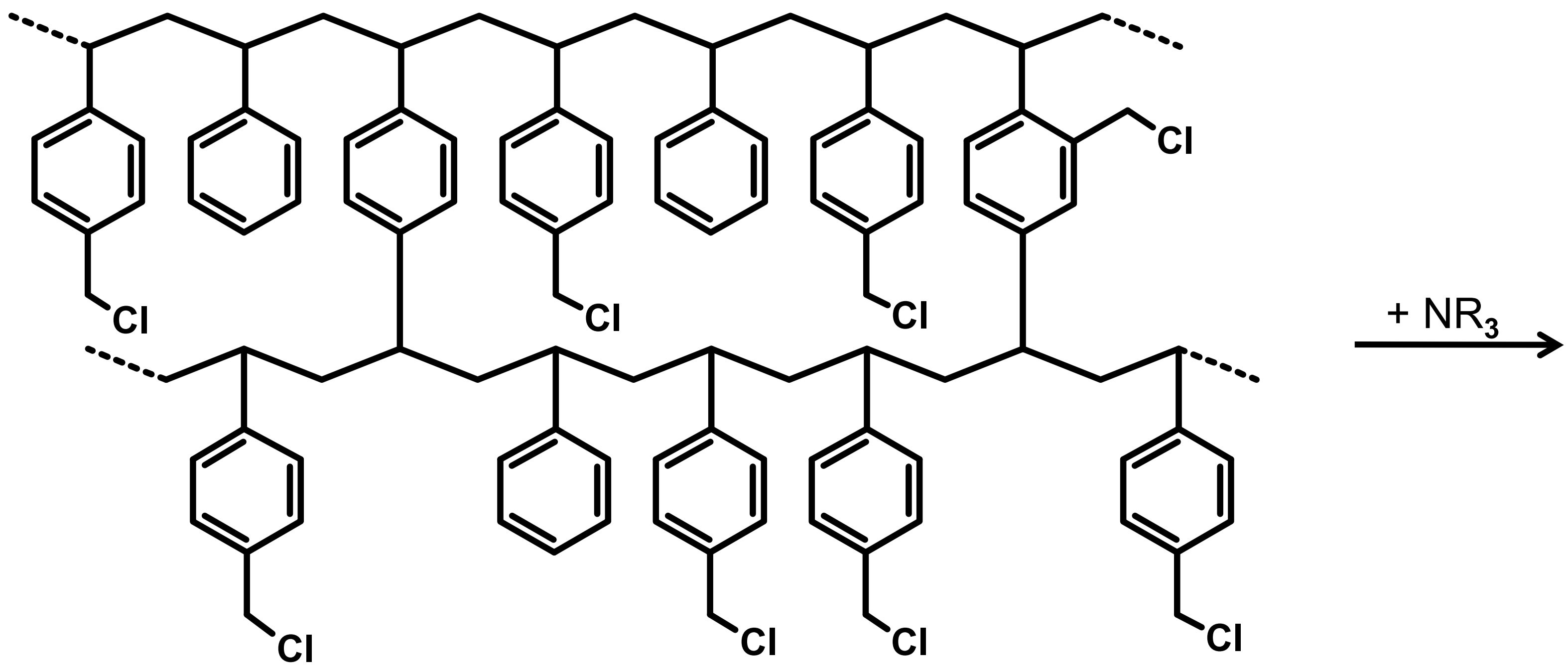
Reaction with a "Lewis Acid"	"Metathesis"-Reaction	Reaction with a "Brönsted Acid"	Reaction at the Ion Exchanger

Technical Synthesis Routes, Anion Exchange Resin.

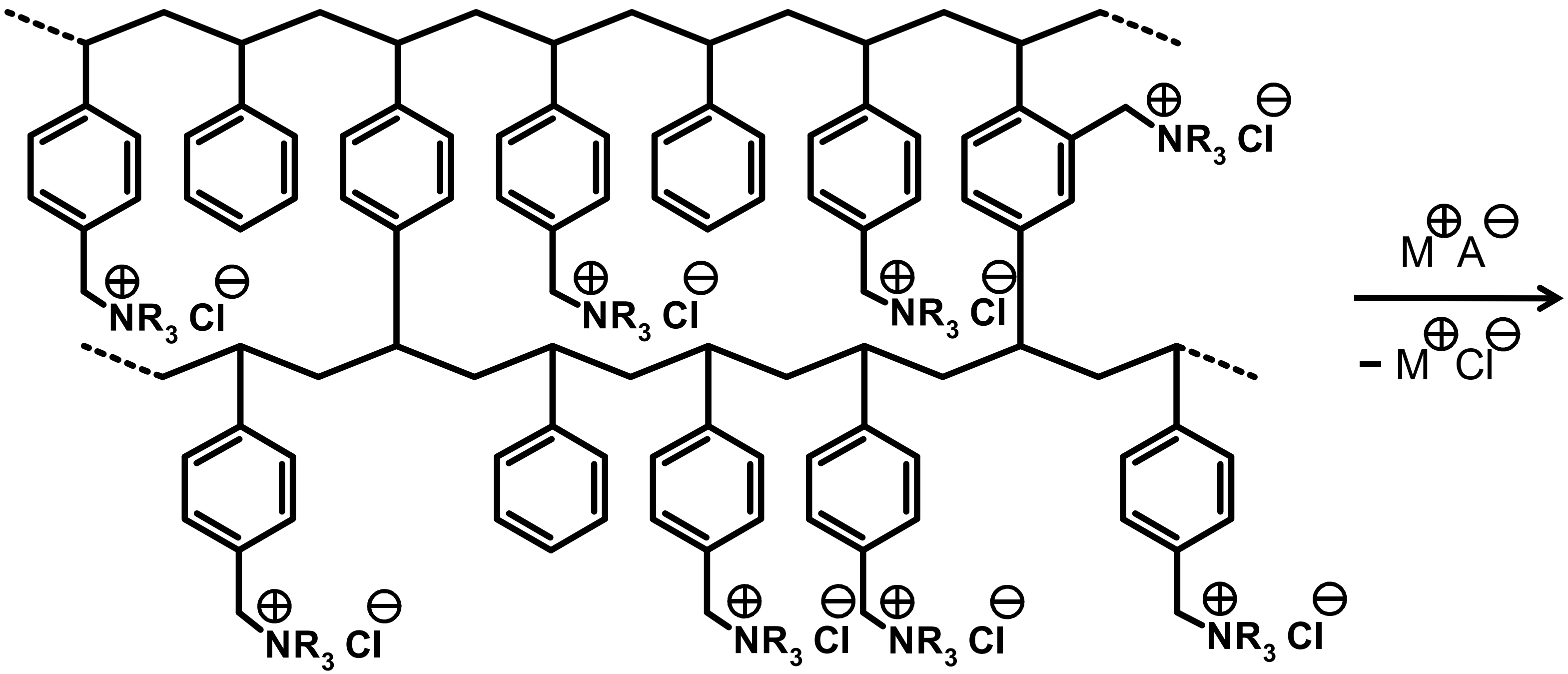




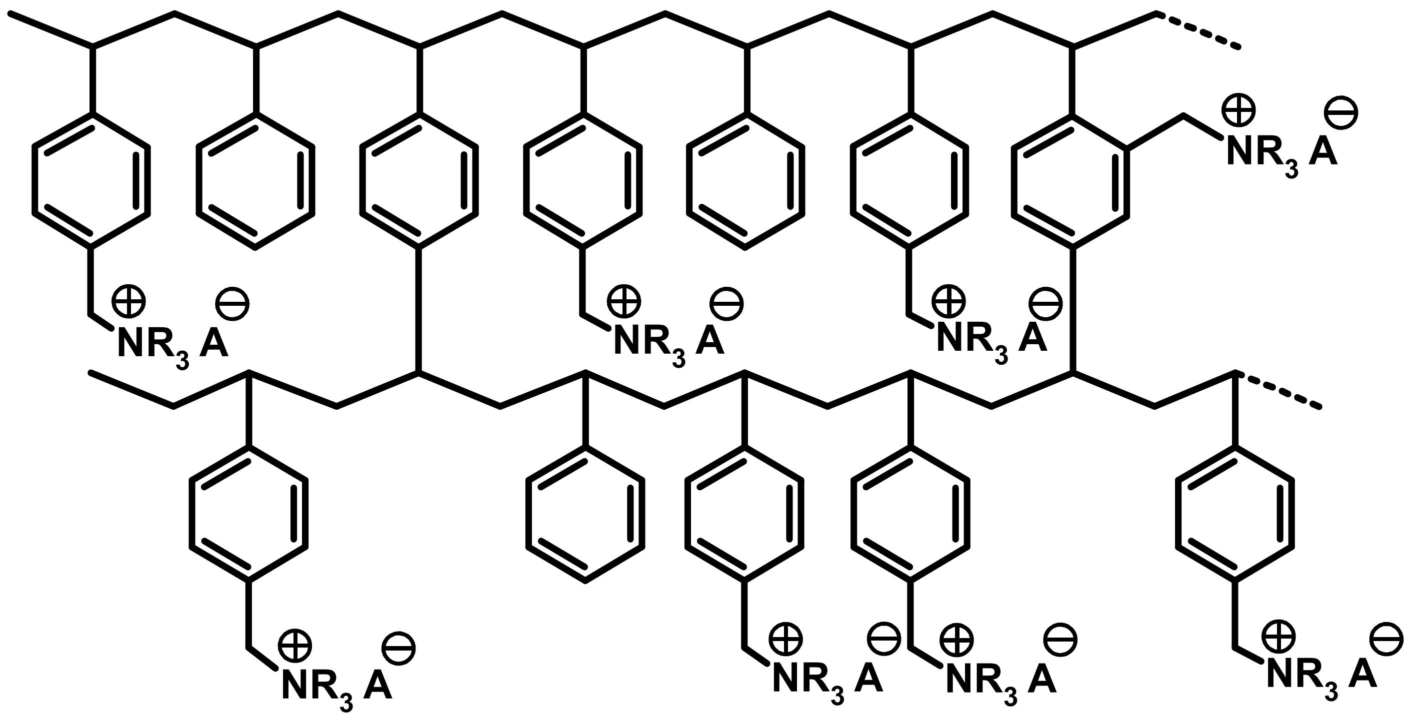
Technical Synthesis Routes, Anion Exchange Resin.



Technical Synthesis Routes, Anion Exchange Resin.



Technical Synthesis Routes, Anion Exchange Resin.



Further Areas of Application in Chemistry and Technology.

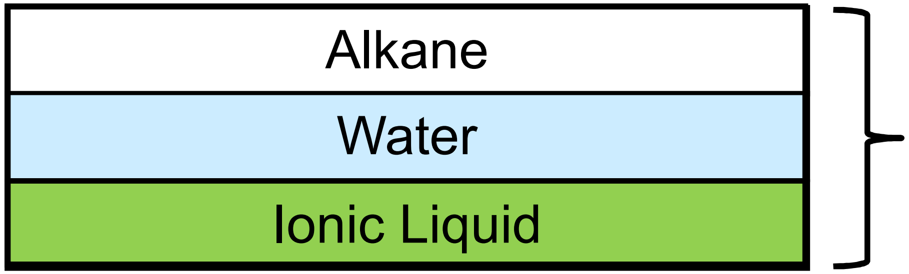
Synthesis and Catalysis.

- "Green" solvents for highly efficient organic reactions or processes.
- Two-phase transition metal catalysts within an ionic catalyst phase.
- Enzyme-catalyzed reactions are possible.
- Biphasic Acid Scavenging utilizing Ionic Liquids.
- Ionic liquids enable the controlled generation of nanoparticles.

Further Areas of Application in Chemistry and Technology.

Synthesis and Catalysis, Procedural Advantages.

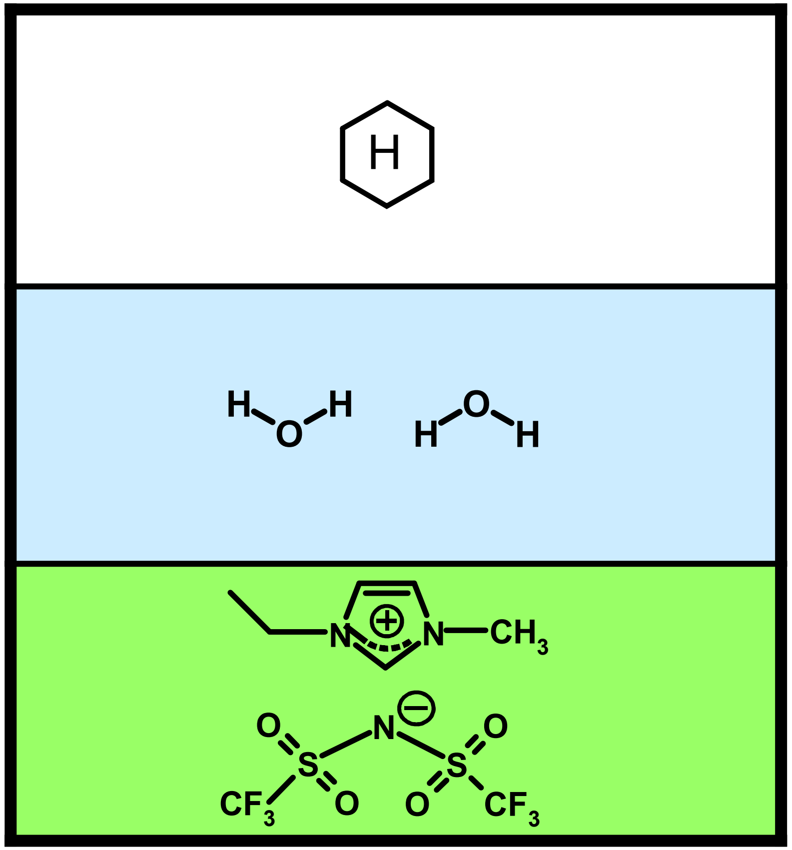
- Ionic liquids allow multiphase reactions.
- Effective isolation of reaction products through simple phase separation.
- The reusability of the applied catalysts is given.



Three-phase system with an intended insolubility of the ionic liquid in water.

Further Areas of Application in Chemistry and Technology.

Example for a Stable Three-Phase System.



Cyclohexane

Water

$EMIM^{\oplus}$ - $(CF_3SO_2)_2N^{\ominus}$

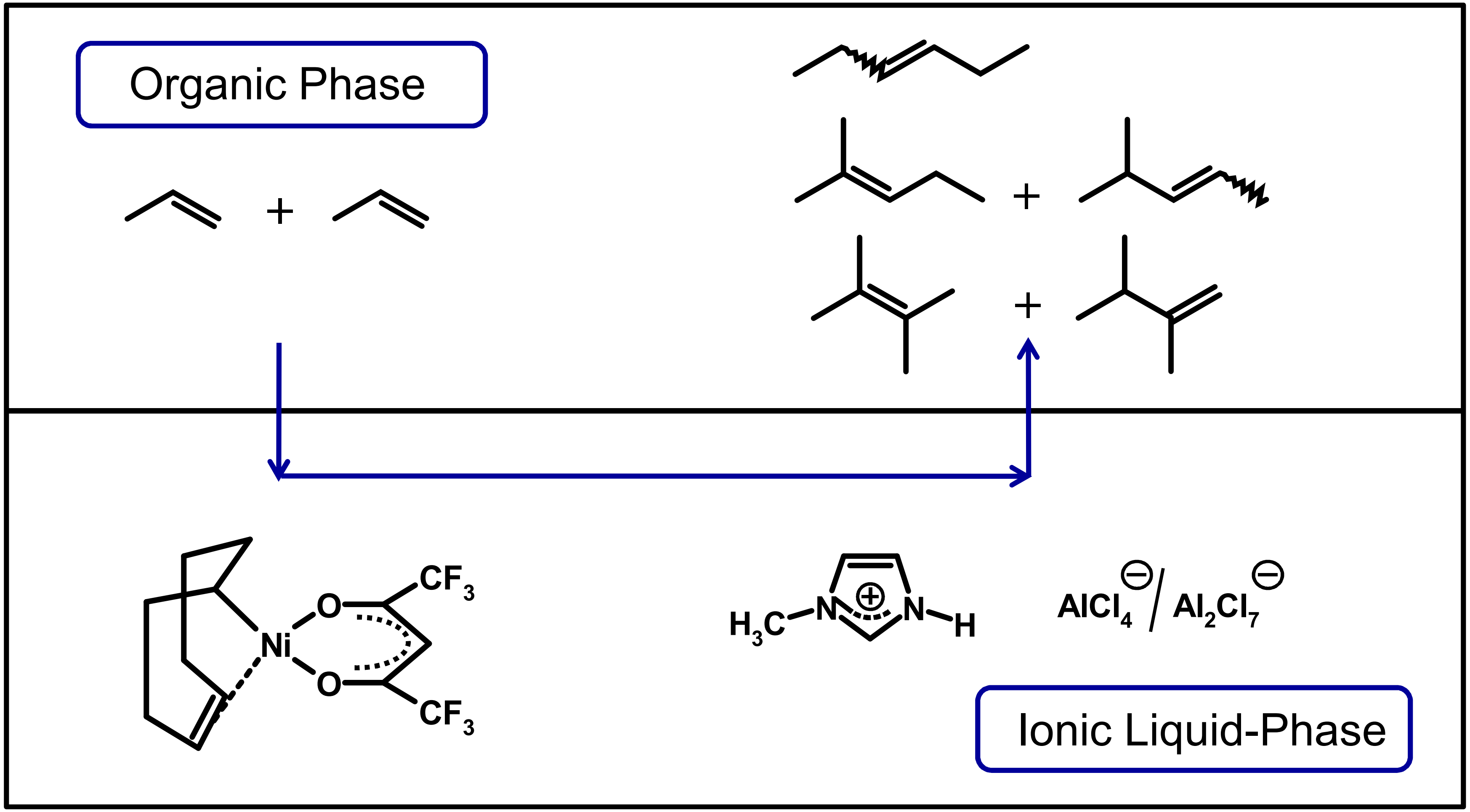
Further Areas of Application in Chemistry and Technology.

Advantages for Process Engineering.

- Elevated reactivity of the reactants.
- Increase in space-time yield.
- Reduction of energy and water costs.
- Improved selectivity of the reaction.
- Reduction in the amounts of raw materials required.
- Reduction of by-products.
- Easier workup of the reaction products.
- Clear separation of the liquid phases.
- Recyclability of the ionic liquid and/or the catalyst.

Further Areas of Application in Chemistry and Technology.

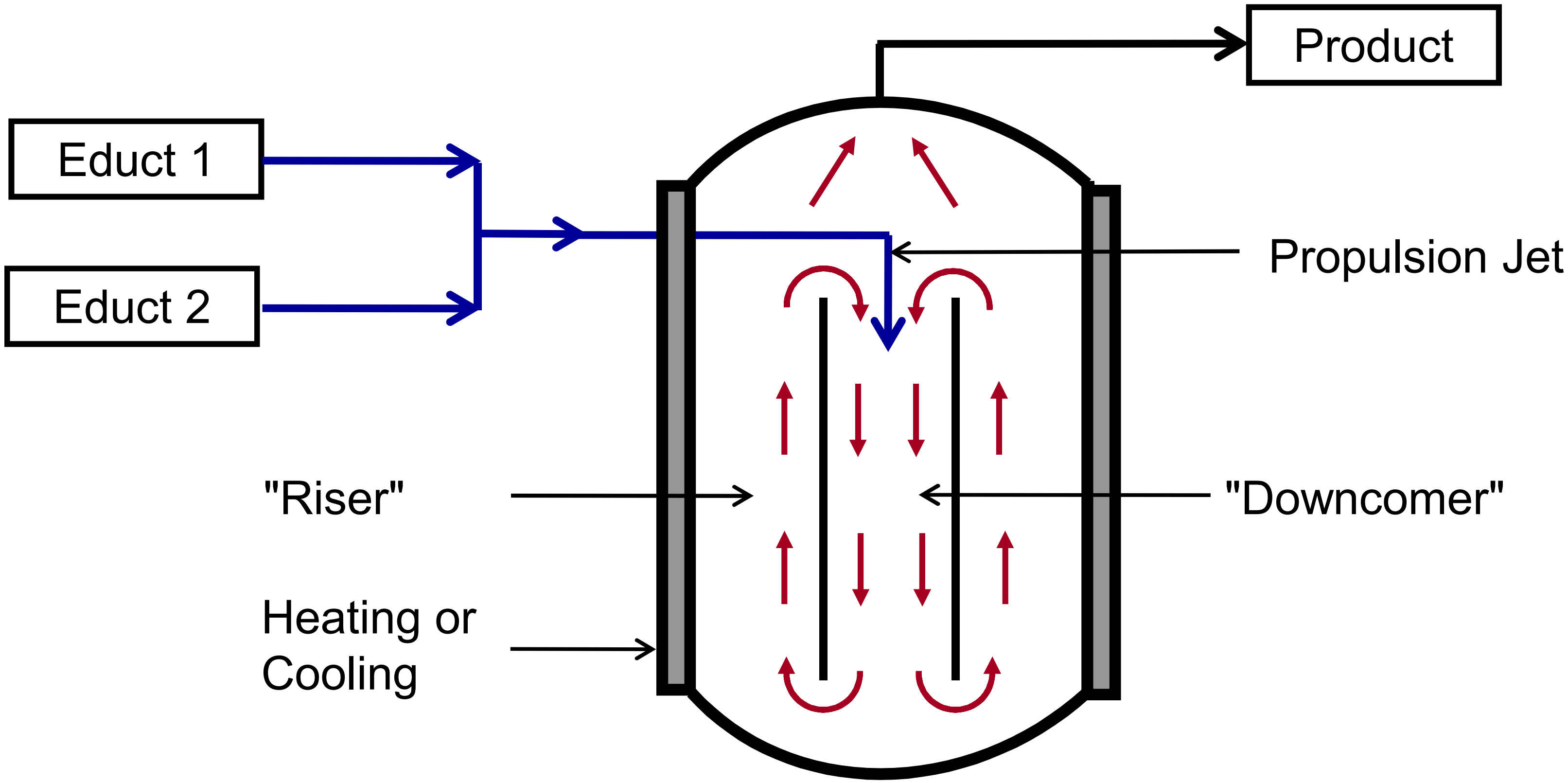
Two-Phase Dimerization of Propene.



Ionic Liquids, Further Fields of Application

Further Areas of Application in Chemistry and Technology.

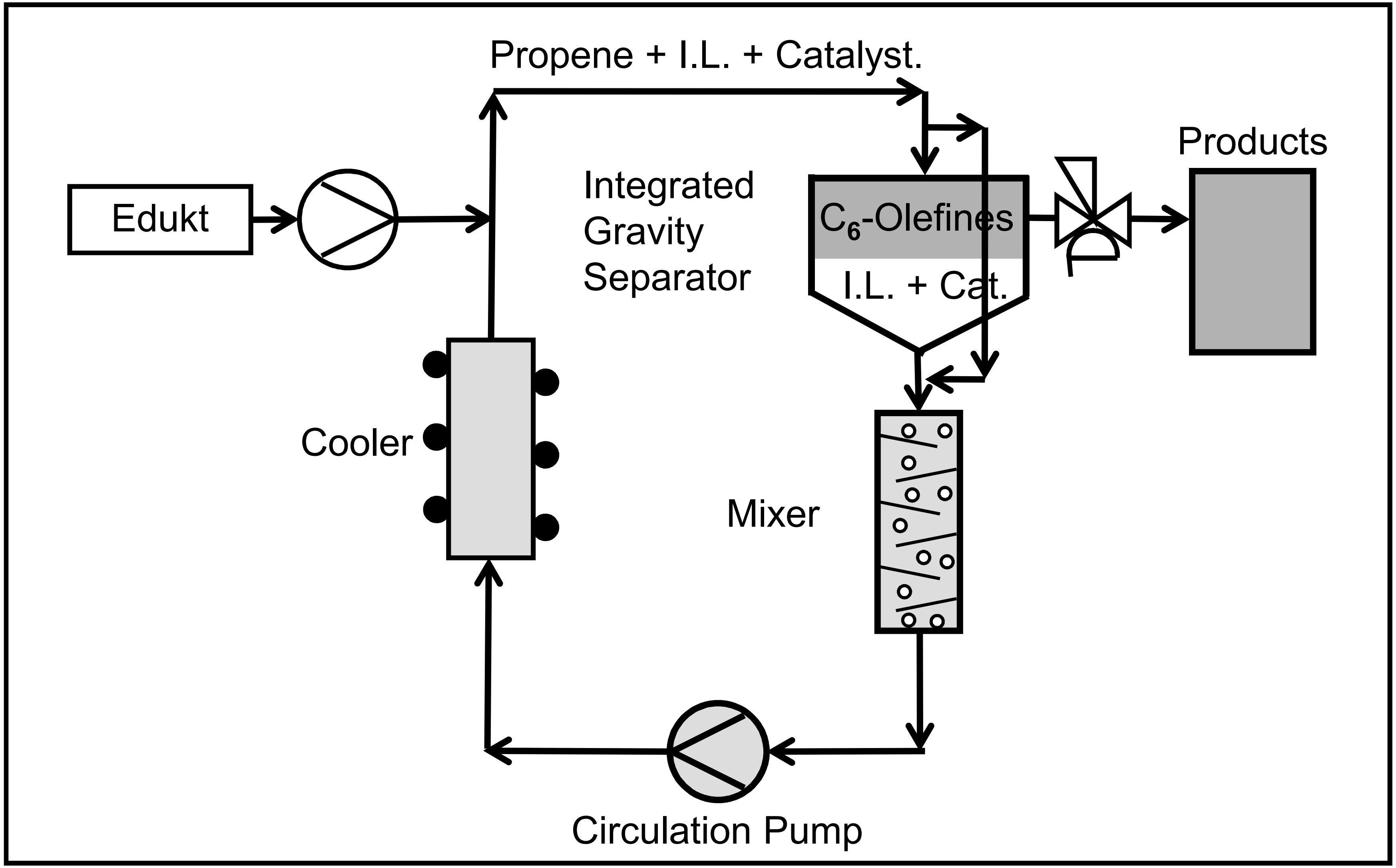
Loop Reactor, Construction, Circular Mode of Operation.



Internal "Double Loop"

Ionic Liquids, Further Fields of Application

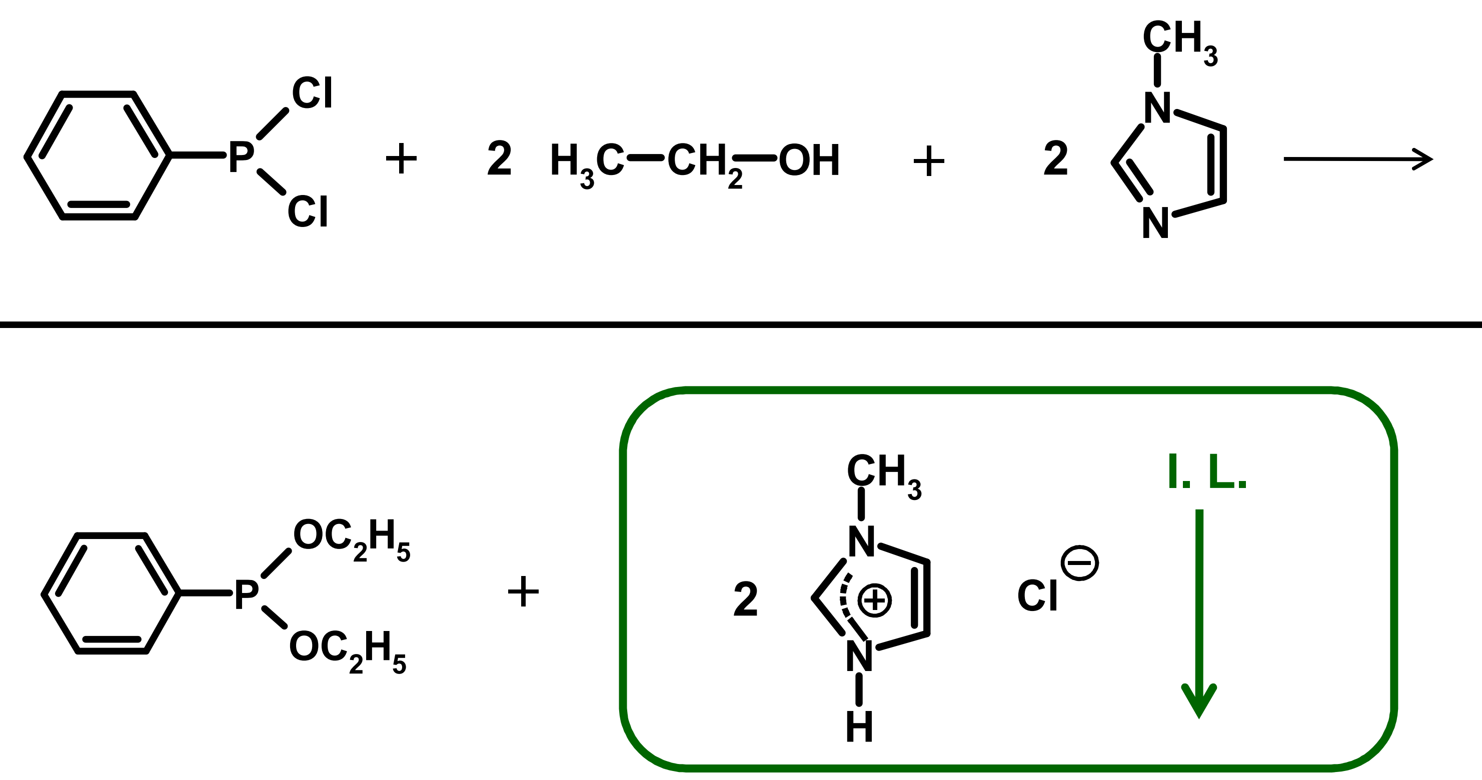
External Loop Reactor, Dimerization of Propene.



Further Areas of Application in Chemistry and Technology.

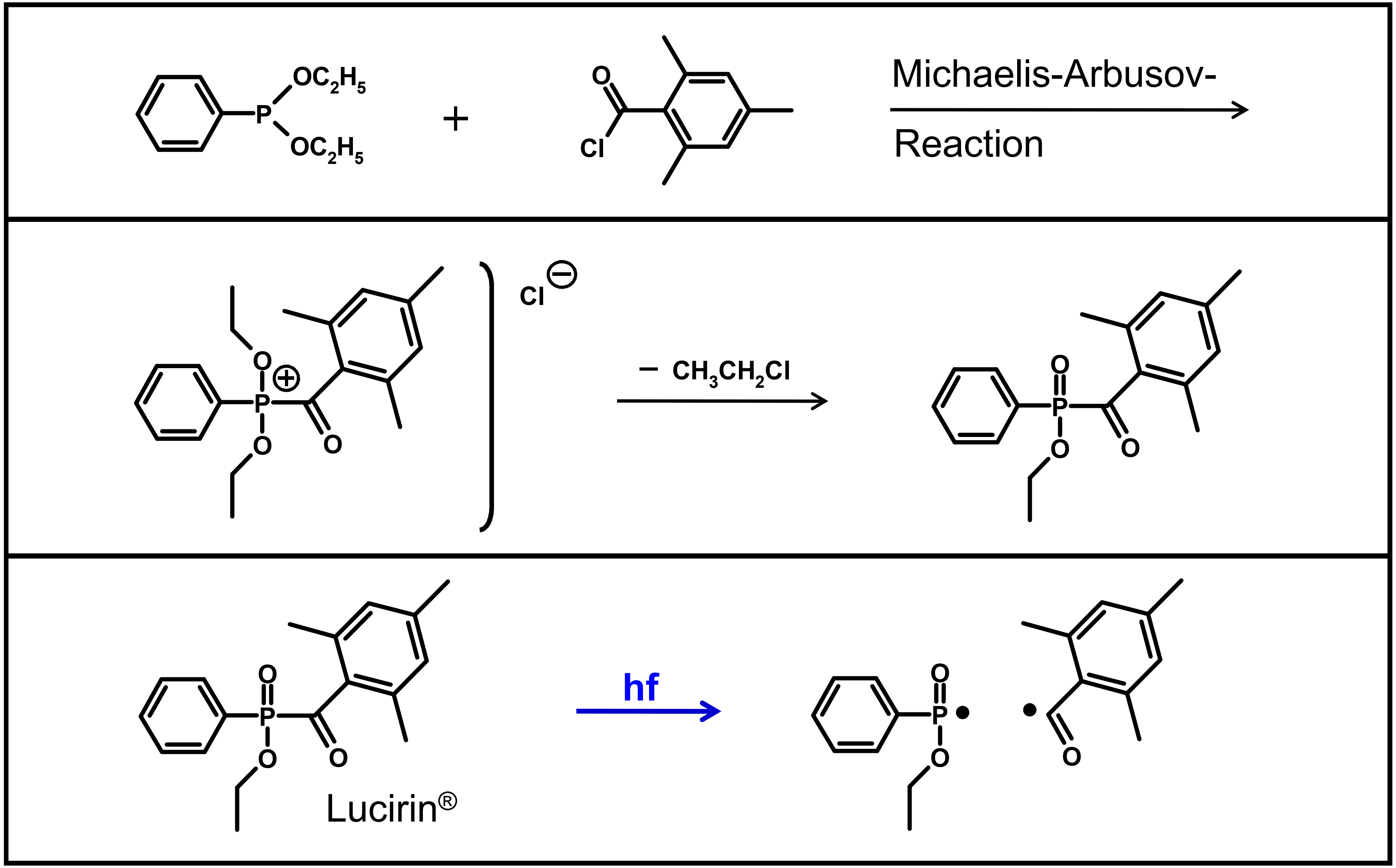
BASIL®-Process from BASF SE.

"**B**iphasic **A**cid **S**cavenging with **I**onic **L**iquids"



Further Areas of Application in Chemistry and Technology.

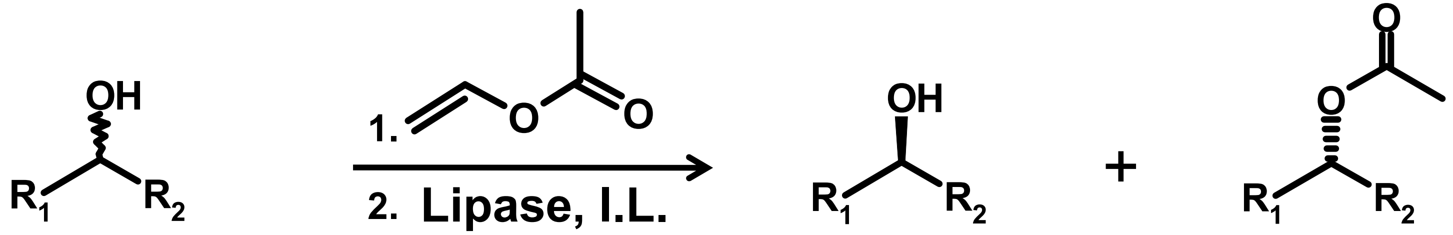
Lucirin®-Synthesis, Decay of the Molecule in UV-Light.

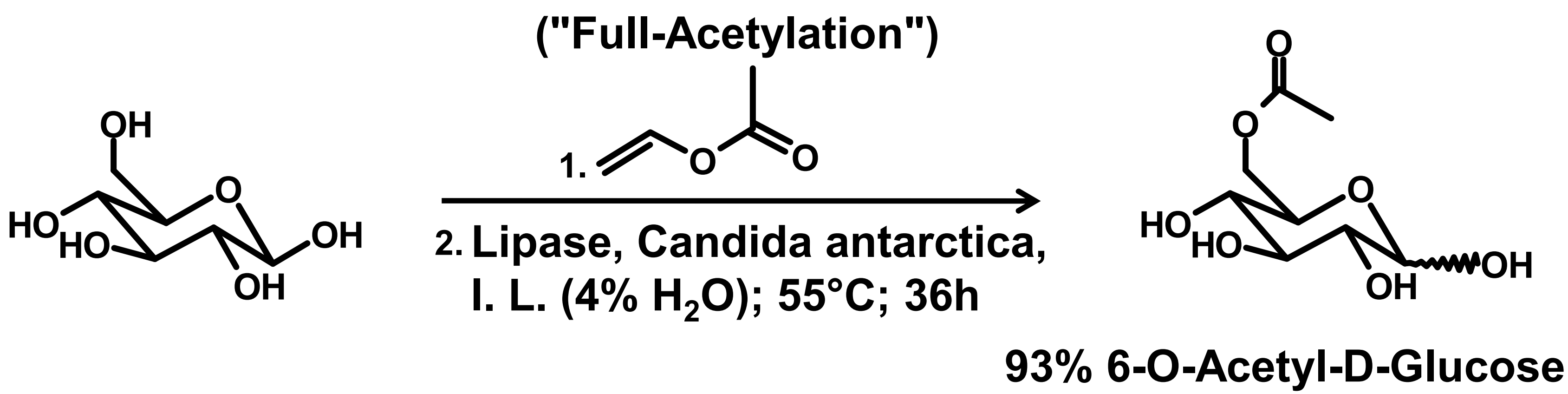


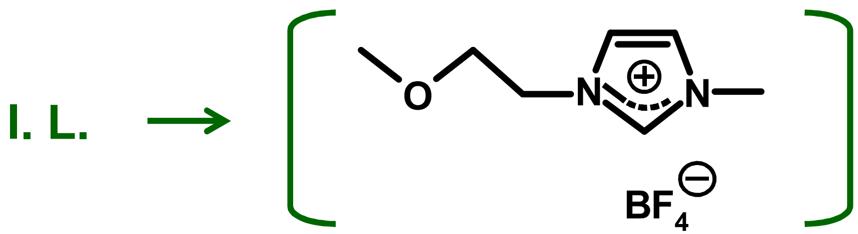
Rainer Buerstinghaus

Further Areas of Application in Chemistry and Technology.

Biocatalysis with the Enzyme Lipase.





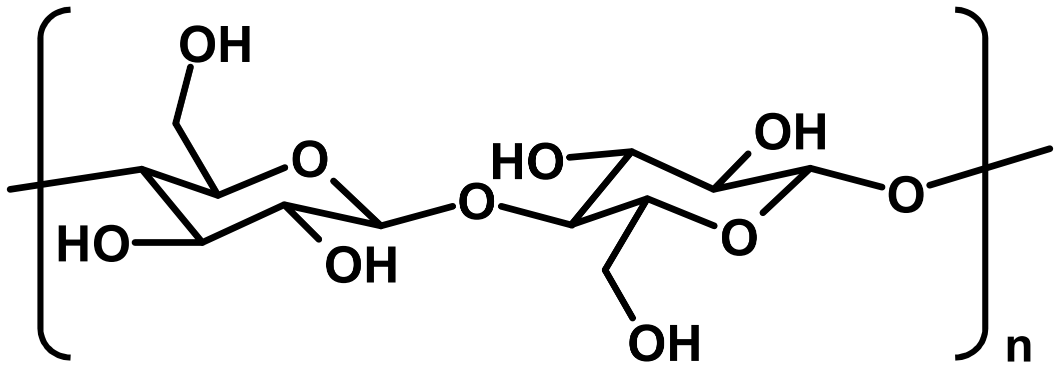


Further Areas of Application in Chemistry and Technology.

"Green Solvent" for Cellulose Macromolecules.

Cellulose, total amount: 700.000.000.000 t on earth.
Natural annual production, worldwide: 40.000.000.000 t.

Several hundred to ten thousand β-D-glucose molecules are (1-4)-β-glycosidically linked together .

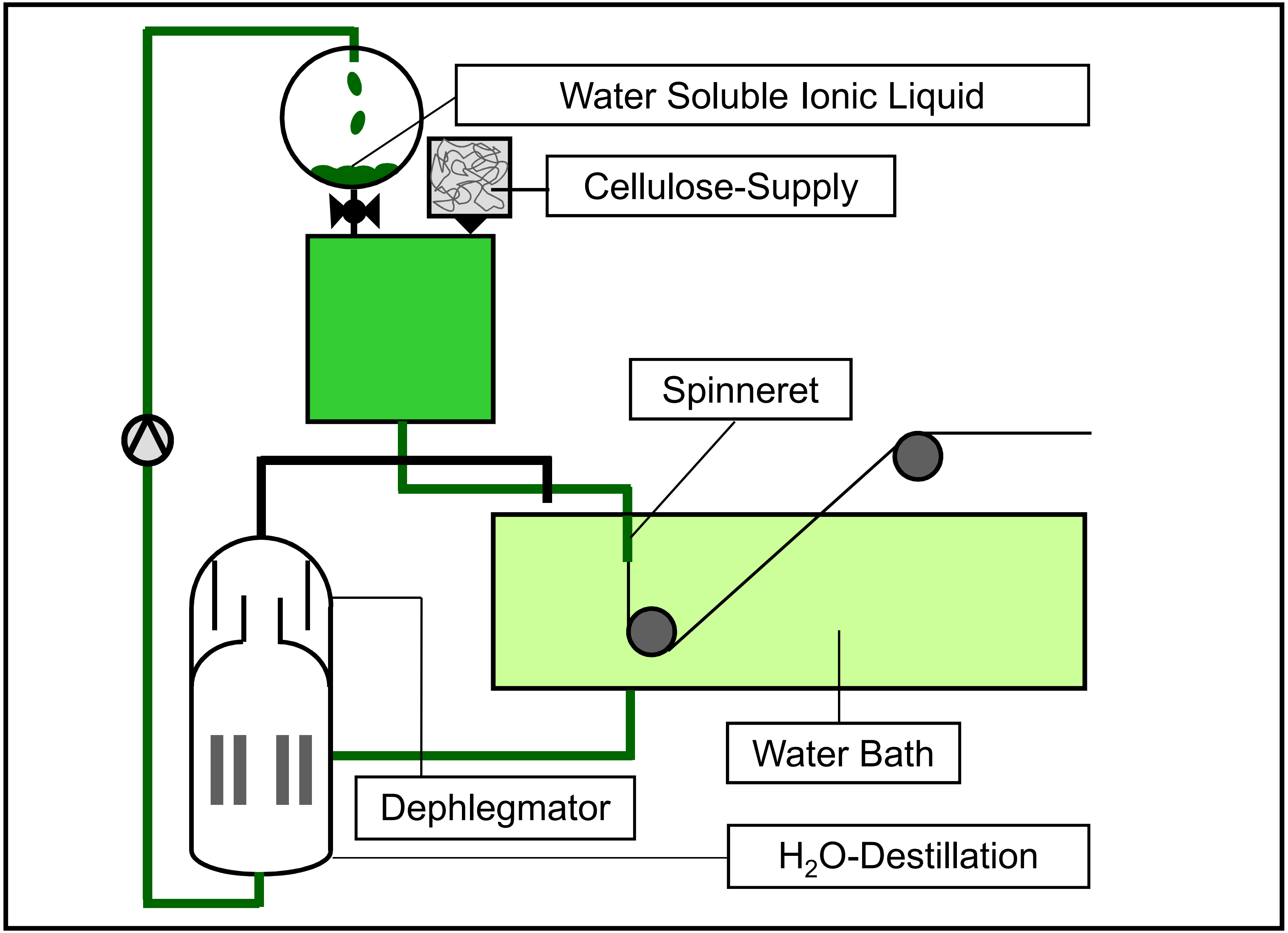


Applications

Basic material in the paper industry (pulp); Clothing industry: viscose; Building materials industry (methyl cellulose) as a flow improver; Packaging industry: cellophane; Toy industry: celluloid.

Rainer Buerstinghaus

I. L.: "Green Solvent" for Cellulose Macromolecules.



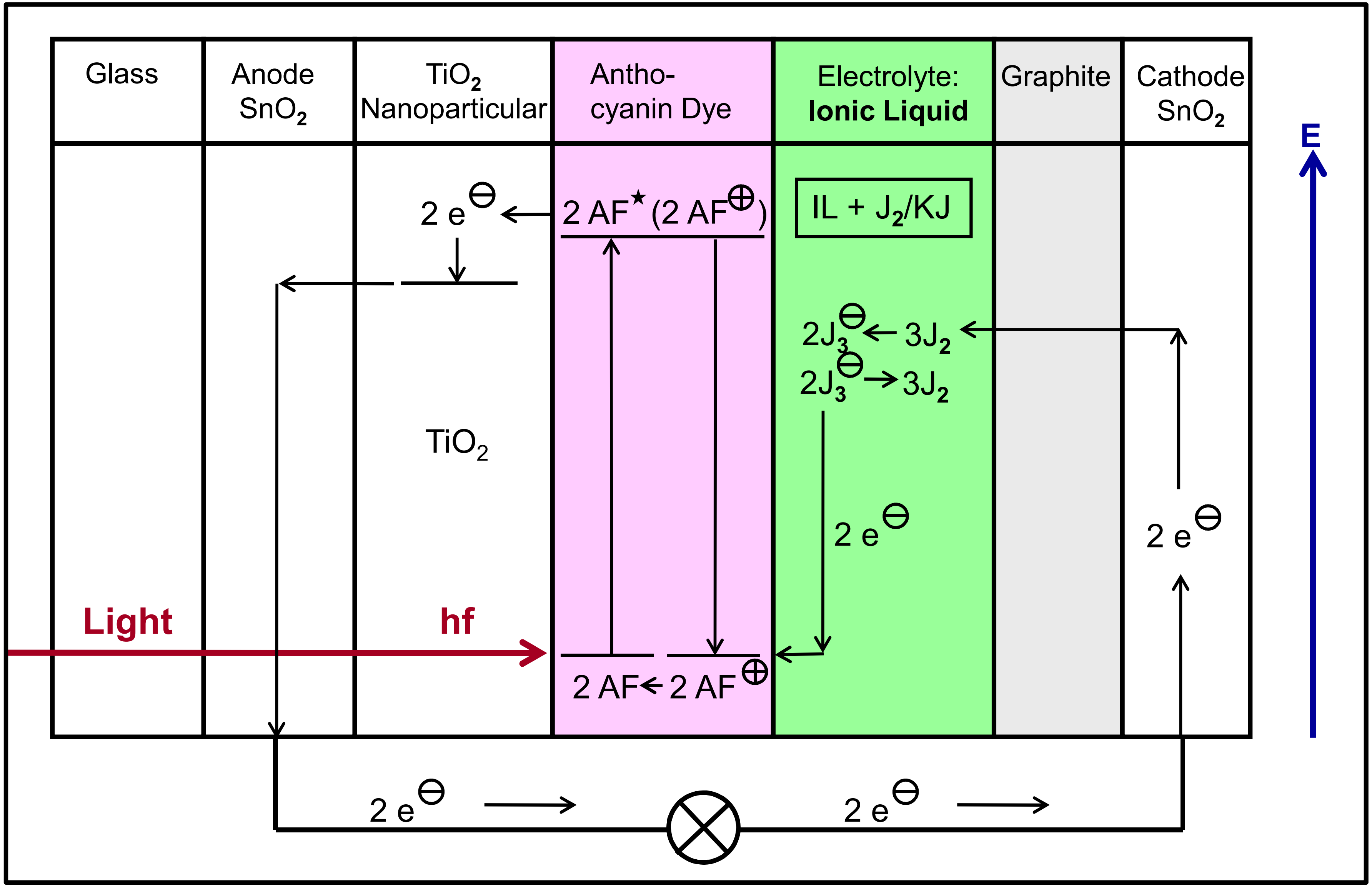
Rainer Buerstinghaus

Further Areas of Application in Chemistry and Technology.

Electrolyte Fluid in Electrical/Electronic Devices.

- Fuel cells for the power electronics and the electric motor of a vehicle.
- Dye solar cells: Grätzel cells.
- Sensors: Humidity sensors, inclination sensors.
- Batteries: Flame-retardant electrolyte liquids for lithium ion batteries.
- Electroplating: Electrical deposition of metals such as Al, Mg, Ti.
- Super capacitors for electronic devices.

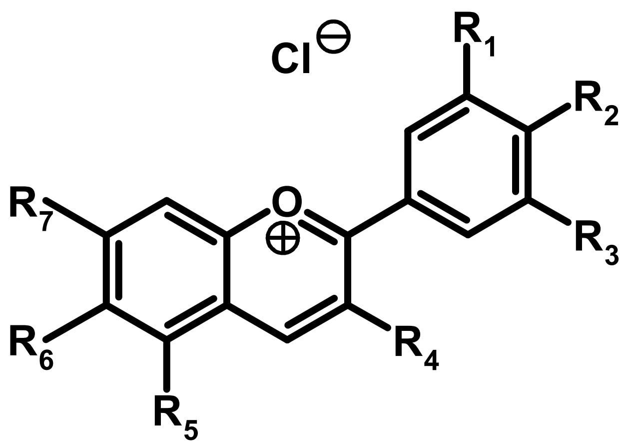
Dye Sensitized Solar Cell (M. Grätzel): Operation Principle.

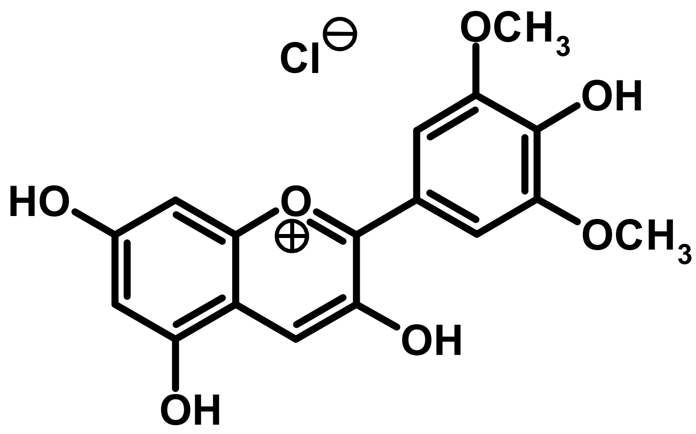


Rainer Buerstinghaus

Dye Solar Cell: Anthocyanins, Chemical Structures.

Greek: άνθος = Flower; κυανεος = Dark Blue



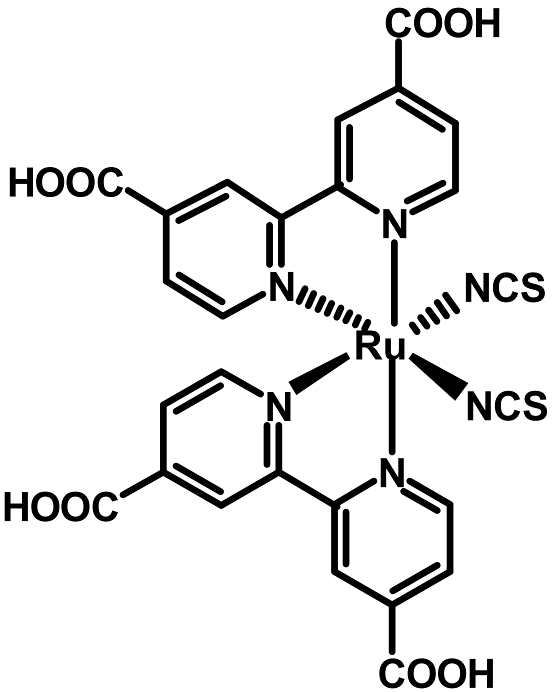


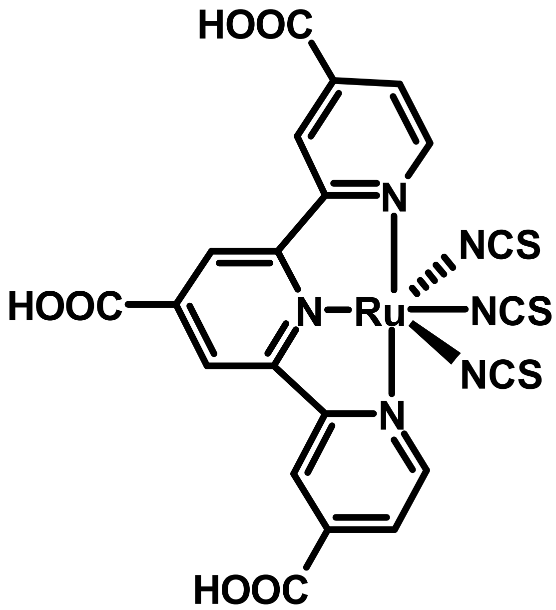
R_1 – R_7 = H, OH, OCH_3

Malvidine

Rainer Buerstinghaus

Dye Solar Cell: N3 and Black-Dye, Chemical Structures.



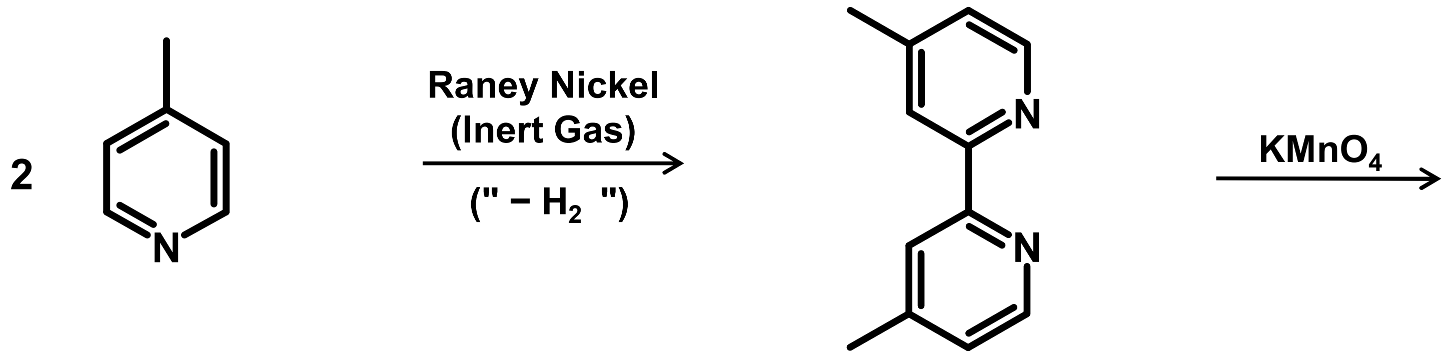


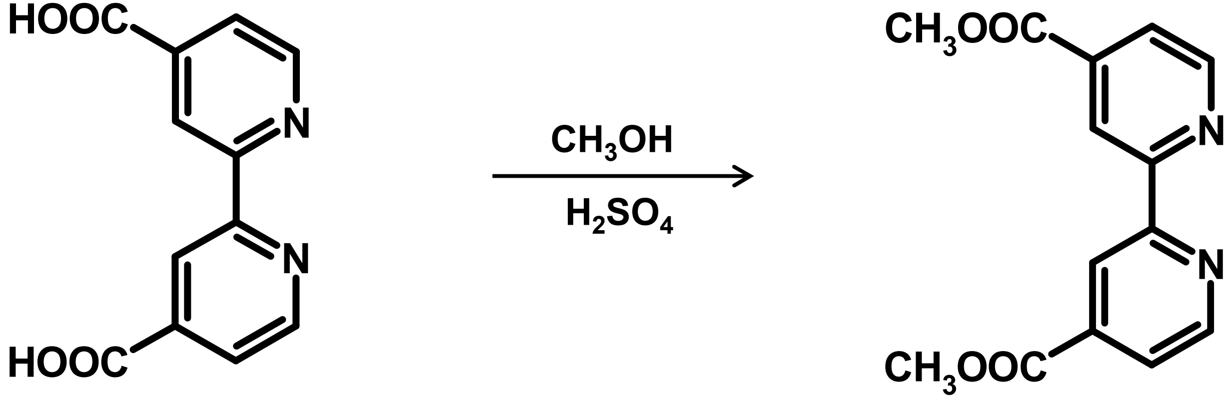
N3	"Black-Dye"

Rainer Buerstinghaus

Further Areas of Application in Chemistry and Technology.

Dye Solar Cell: Synthesis of the N3 Building Block "dmcb".



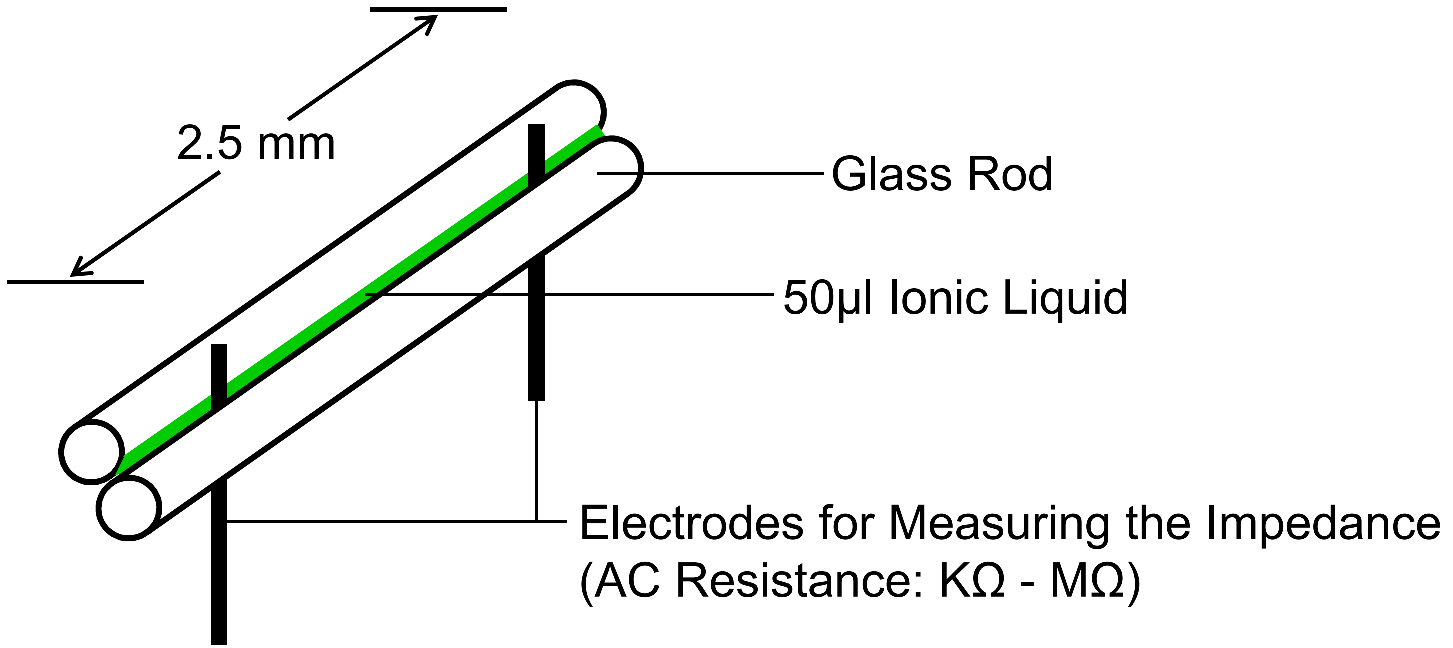


Rainer Buerstinghaus

Ionic Liquids, Further Fields of Application

Further Areas of Application in Chemistry and Technology.

Electrolytes: Humidity Sensor According to Novasina S.A.



The AC resistance increases with increasing relative humidity.
Advantage: Short response times.

Rainer Buerstinghaus

Further Areas of Application in Chemistry and Technology.

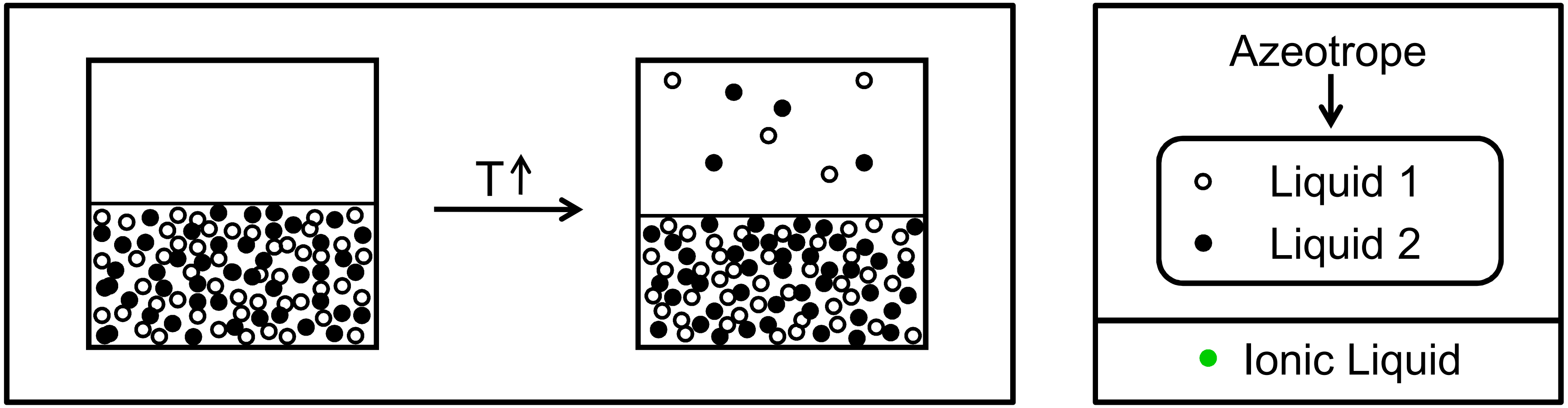
Separation Technology, Release Agents, Additives.

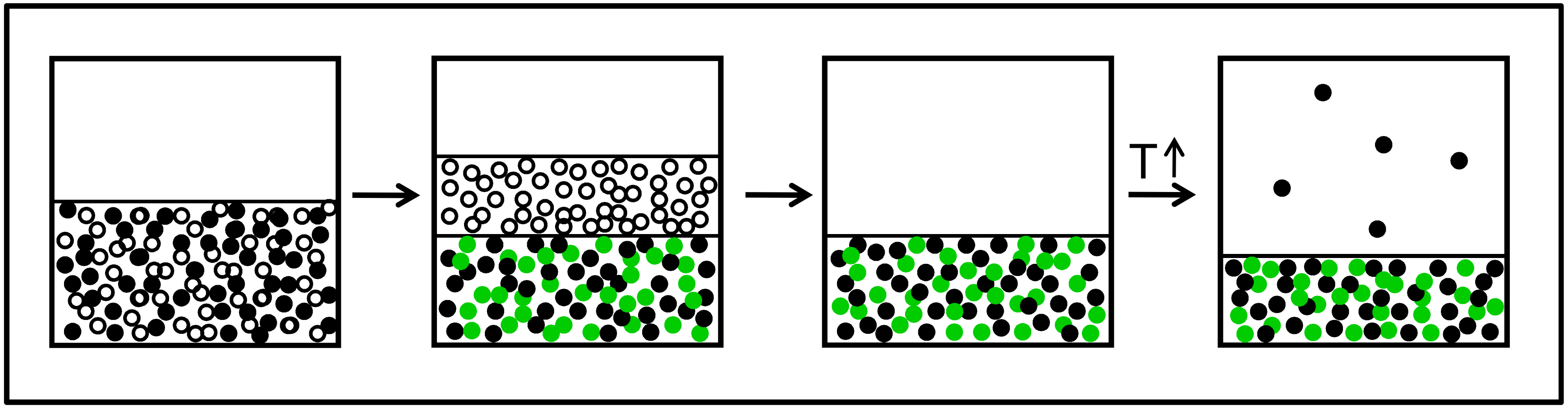
- Gas separation procedures.
- Azeotrope, separation of constituents.

- Cooling liquids and hydraulic fluids.
- Antistatic additives.
- Separation liquids for plastic and metal injection molding.

Ionic Liquids, Further Fields of Application

Ionic Liquids, Area of "Azeotrope Separation".

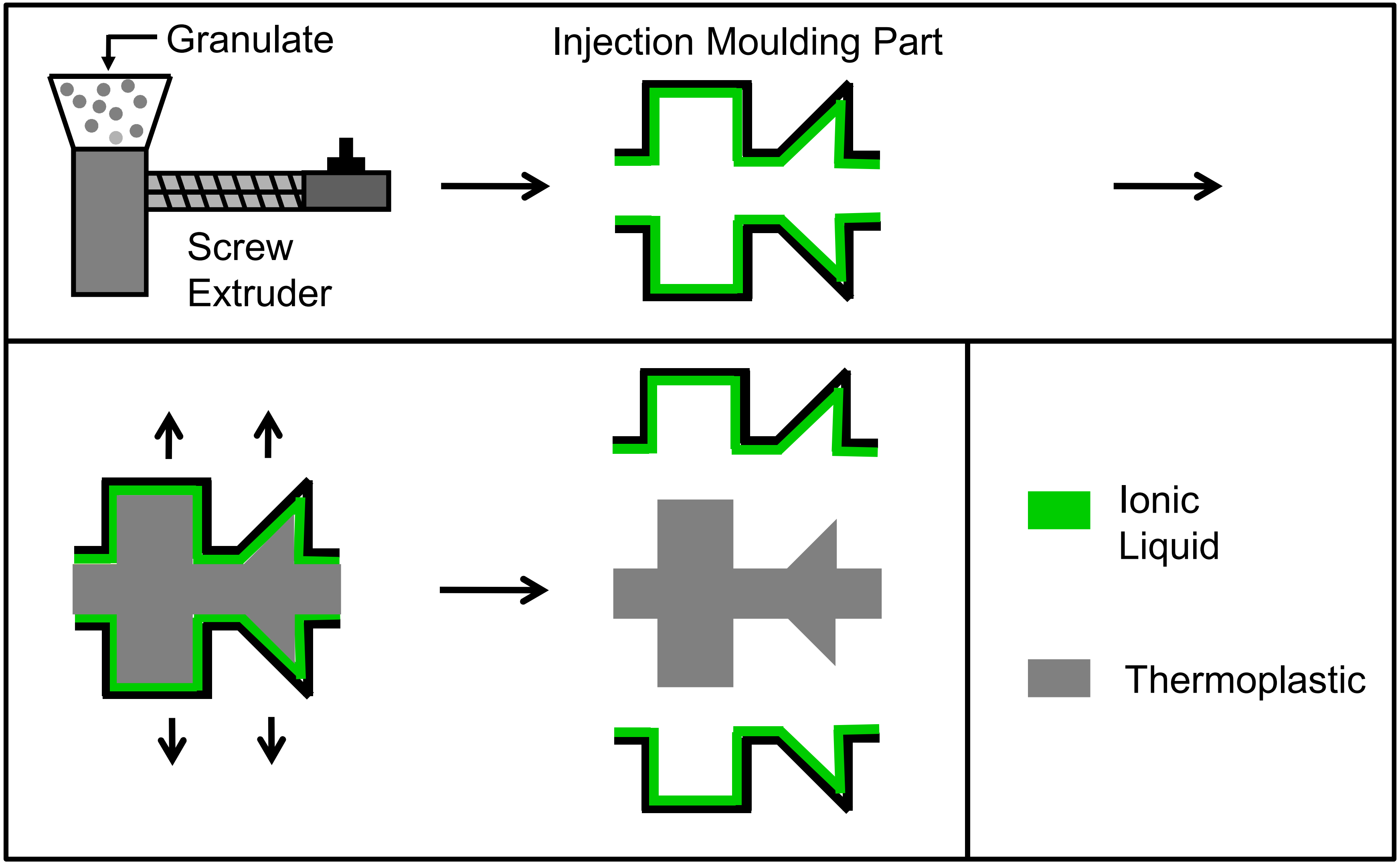




Rainer Buerstinghaus

Ionic Liquids, Further Fields of Application

Ionic Liquid: Application Area "Plastic Injection Molding".



Rainer Buerstinghaus

Ionic Liquids, Application Areas in Chemistry and Technique: Liquid Crystals, Electro-Elastic Materials, Heat Transfer and Storage.

- Displays: TV; PC`s; Mobile phones.

- Artificial muscles.

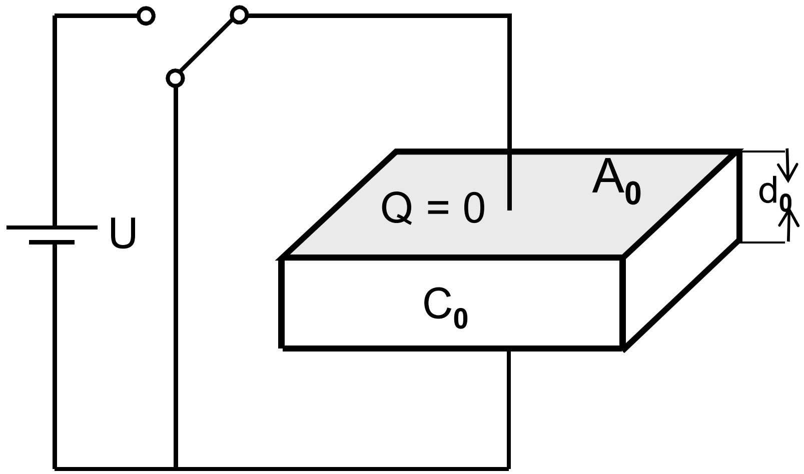
- Thermal fluids: Heat transfer media.
- Cryo fluids: cold sorptive media.
- Phase change media (PCM).

Ionic Liquids, Further Fields of Application

Application Area "Electro-Elastic Materials".

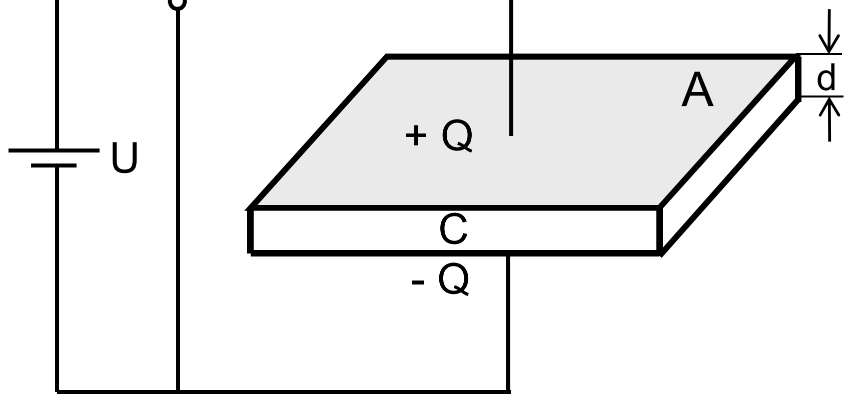
EAP-Actuator (Electro Actice Polymers $\longrightarrow$ Adaptronics).

Short Circuit



$C_0 = \varepsilon_0 \varepsilon_{rx} A_0/d_0$

Activation

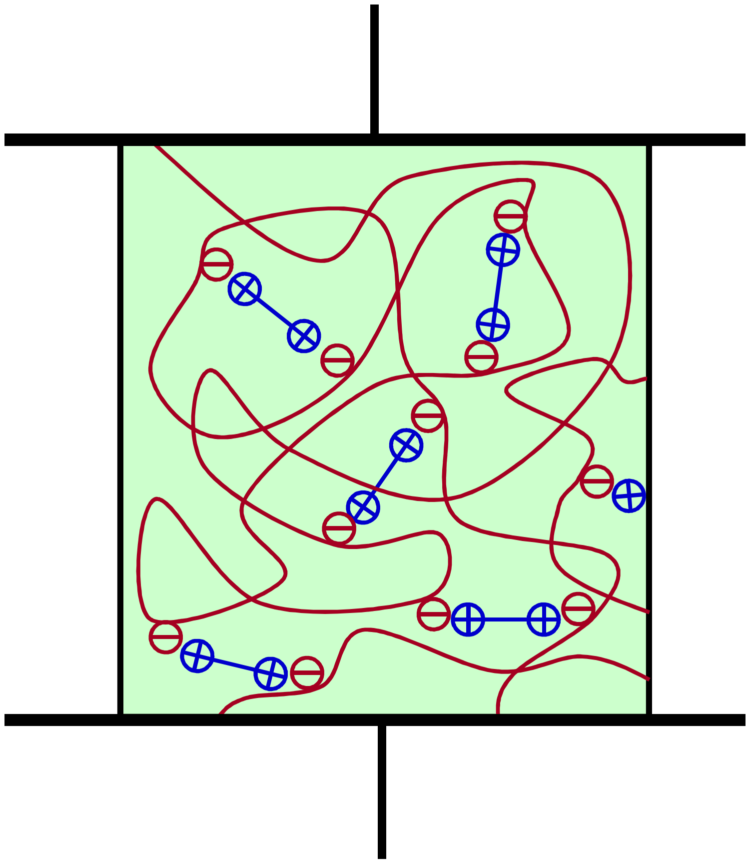


$C = \varepsilon_0 \varepsilon_{ry} A/d$

Ionic Liquids, Further Fields of Application

Application Area "Electro-Elastic Materials".

EAP-Actuator Basing on an Ionic Gel.

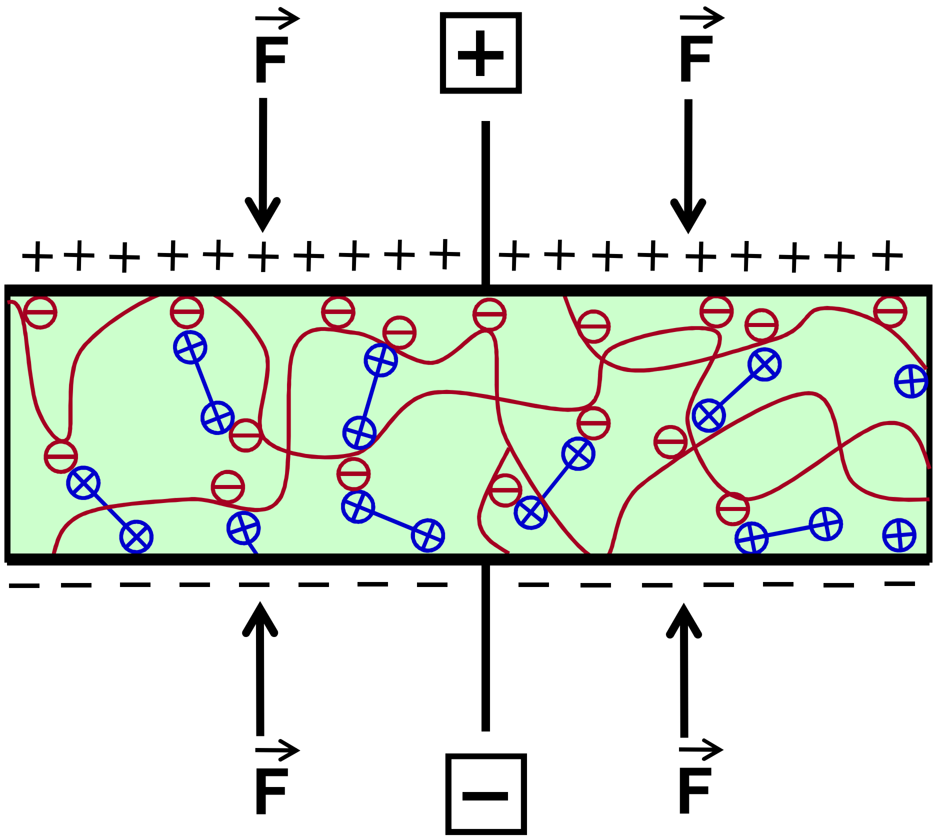


Two capacitor plates:
In between is a gel consisting of an ionic liquid, a negatively charged polyelectrolyte and a bis (ammonium) compound.

Ionic Liquids, Further Fields of Application

Application Area "Electro-Elastic Materials".

EAP-Actuator Basing on an Ionic Gel.



Electric charging:

Force generation through electro-static attraction or repulsion.

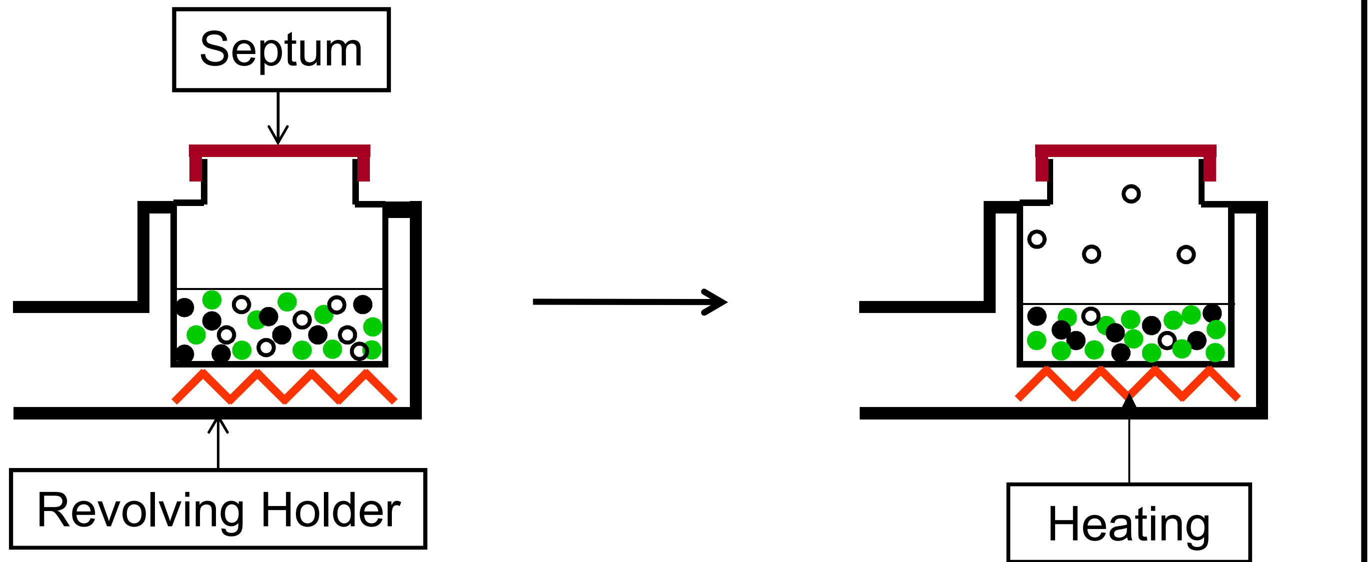
Further Areas of Application in Chemistry and Technology.

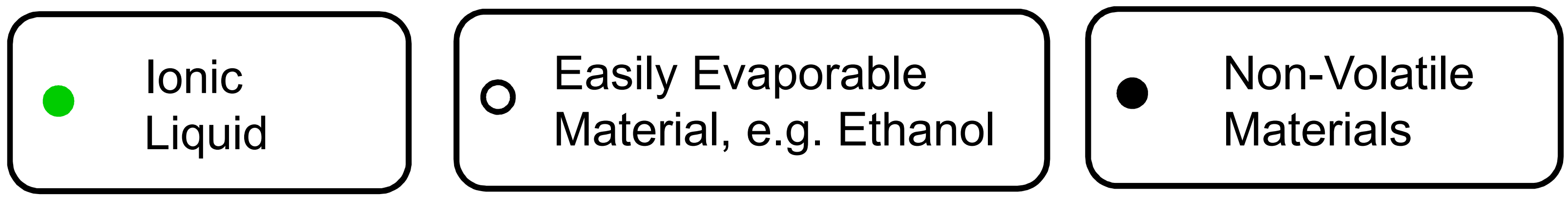
Analytics: Separation, Purification and Determination.

- Solvent for GC head space devices.
- Matrix materials for MALDI-TOF-MS.
- Solvent for Karl Fischer titrations.
- Media for protein crystallization.

Ionic Liquids, Further Fields of Application

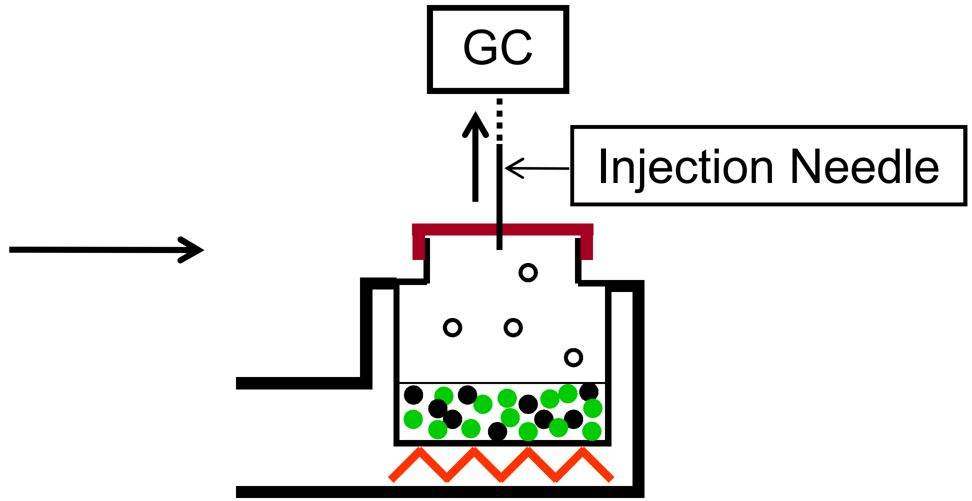
Headspace-GC, Functional Principle.





Rainer Buerstinghaus

Headspace-GC, Functional Principle.



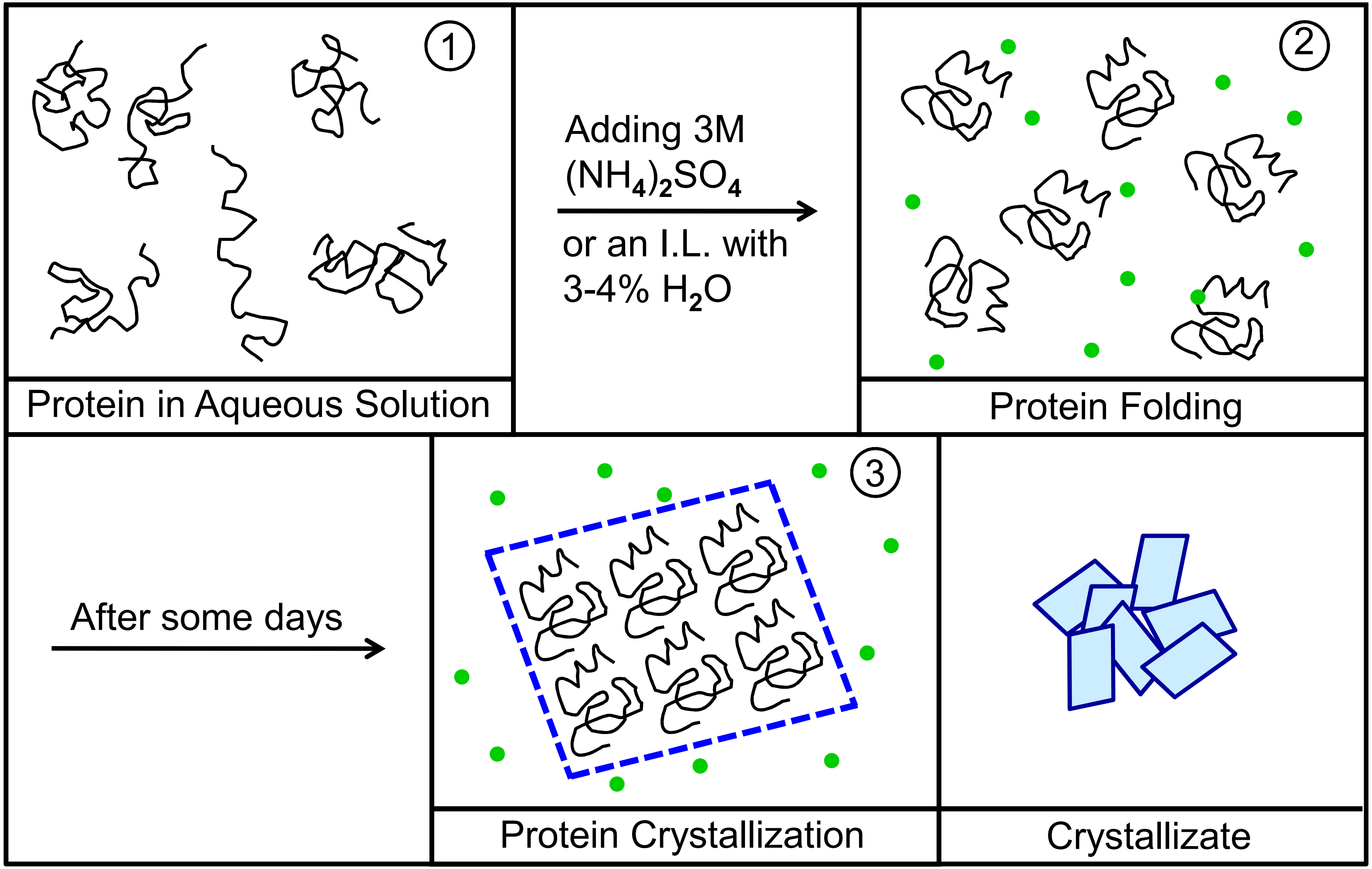
This method can be used to determine the alcohol content in blood samples.

Reference Material: tert-Butanol.

- Ionic Liquid
- Easily Evaporable Material, e.g. Ethanol
- Non-Volatile Materials

Ionic Liquids, Further Fields of Application

Protein Crystallization by Adding an Ionic Liquid.



Rainer Buerstinghaus

R&D Project Management
in the Chemical Industry

End of Supplementary Module 03

Rainer Buerstinghaus