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IUPAC Recommendations

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Glossary of terms relating to electronic, photonic and magnetic properties of polymers (IUPAC Recommendations 2021)

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Abstract: These recommendations are specifically for polymers and polymer systems showing a significant response to an electromagnetic field or one of its components (electric field or magnetic field), *i.e.*, for electromagnetic-field-responsive polymer materials. The structures, processes, phenomena and quantities relating to this interdisciplinary field of materials science and technology are herein defined. Definitions are unambiguously explained and harmonized for wide acceptance by the chemistry, physics, polymer and materials science communities. A survey of typical electromagnetic-field-responsive polymers is included.

Keywords: Electric properties; functional polymers; magnetic properties; molecular electronics; optical properties; organic electronics.

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1 Introduction

The physical and chemical properties of electronically, electro-optically, and opto-electronically active polymers are being increasingly investigated for scientific study, technological development and commercialization. In view of the rapid development and increasing number of applications of polymers as active functional materials in the construction of electronic and optoelectronic devices such as diodes, light-emitting diodes, switches, photovoltaic cells, analytical sensors, batteries, optical fibers, *etc.*, a need for effective and clear communication among chemistry, polymer physics and materials communities is of increasing importance.

Some of the terms commonly used in this interdisciplinary field are of recent development and are indicative of the rapid growth in this area. Other, older terms arise due to the useful, if occasionally erroneous, adaptation of terms developed for inorganic semiconductors. The latter field is more mature, for example inorganic transistors have been available since the 1950s, and the language used to develop an understanding of electronic and optical behaviors was developed with works published from the late 1960s on [1]. The terms of this inorganic-based science thus arose with physicists and inorganic chemists working in tandem.

The considerable development of conducting and semiconducting polymers, through the works of Berets *et al.* in 1968 [2] and, notably Shirakawa *et al.* in 1977 [3], made it possible to start understanding the properties of these materials, for example, their charge transport capability and susceptibility to doping, and their electronic and optical behaviors [4–6]. In this field, however, due to the large number of structures that can be considered and made accessible by organic and organic-inorganic polymer chemistry, and the as yet incomplete understanding of the physics of what are often (although not exclusively) conjugated polymers, there are still uncertainties of the actual underlying processes. Furthermore, this area brings together an extraordinarily wide range of scientific disciplines, ranging from synthetic polymer chemistry, through physics to materials science.

Given this current state of affairs, there is a need to define terms that provide common ground for the divergent groups of specialists working in this area. Furthermore, there is a secondary objective of clarifying the similarities and differences in the physical processes underlying the fields of polymer- and inorganic-based materials and devices.

In summary, it is the aim of these IUPAC Recommendations to provide chemists, physicists and material scientists with a useful glossary that can facilitate their interdisciplinary communication and help them to understand the rationale underlying the terms and their definitions which originate from various fields of science and technology. The authors hope that the glossary will help to harmonize understanding of identified terms specific to field-responsive polymers and enforce correct use of these terms by the people active in the field.

In the first section of the glossary, the structure, properties and processes related to electronic, electro-optic, and opto-electronic related polymers are defined and elaborated. Particular attention is paid to the definitions of terms used in other, closely related topics *viz.* the use of terms such as soliton and polaron on the one hand, and delocalized radical, ion and radical-ion on the other. In such instances, both chemical and physical viewpoints are presented and explained. In the second section, further insight is provided through a survey of classes and typical examples of polymers that are currently used within this field.

2 Terms relating to structure, properties and processes

2.1 action spectrum

responsivity spectrum

Graphical dependence of the relative photoresponse of a system on the wavelength, or wavenumber, or photon energy of the incident irradiation at the same radiant power of light [7]; modified.

Note 1: The photoresponse can be of physical, chemical, biological or physiological nature.

Note 2: Ideally, the *quantum yield* of photoresponse (the number of response events per number of incident photons) should be plotted in an action spectrum. However, the spectra normalized to the maximum photoresponse are often used since they point to the most efficient incident irradiation.

2.2 actuator

Transducer that converts the energy supplied or taken from the surroundings into some mechanical motion.

Note: Human muscles, motors, loudspeakers and various piezoelectric devices are examples of actuators.

2.3 antisoliton

Soliton with the negative amplitude or opposite spin with respect to a given *soliton* [8].

2.4 bandgap energy

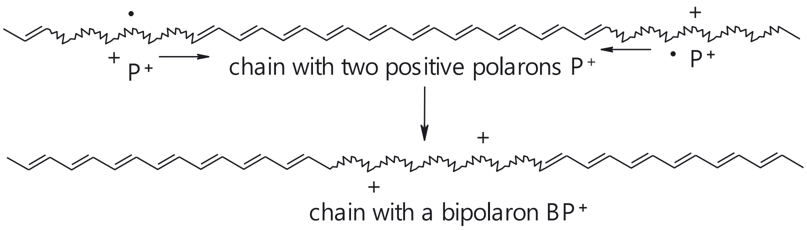
Energy difference between the bottom of the *conduction band* and the top of the *valence band* in a *semiconductor* or an *insulator* [7].

Note: Bandgap energy generally dictates the electronic and optical properties of molecules and materials.

2.5 bipolaron

Quasiparticle consisting of two *polarons* sharing the same *lattice* distortion [8, 9]; modified.

Note 1: A bipolaron is a spinless double charged *quasiparticle* with boson properties.
Note 2: Each *polaron* is associated with a local *lattice* distortion that causes internal stresses in the system. If two *polarons* of the same charge sign occur in proximity, they can start share the same distortion by releasing unpaired electrons into a molecular orbital extended over the shared distortion. Binding of two *polarons* into one bipolaron is effective, because the decrease in the number of distortions reduces the system energy so much that it outweighs the Coulombic repulsion of nearby charges.



2.6 charge carrier

Particle or *quasiparticle* capable of transporting an electric charge.

Note 1: Examples of charge carriers are *electrons, electron holes*, protons or other ions, charged *solitons*, *polarons* or *bipolarons*.
Note 2: A charge carrier can be free (mobile) or trapped (immobile).
Note 3: See also *Coulomb radius*.

2.7 charge carrier
concentration of charge carriers

Number of *charge carriers* per unit volume [10].

Note: A use of the term "charge carrier density" is depricated since it can easily be confused with the term *charge density* whose meaning is different, see entry 2.13.

2.8 charge carrier diffusion

Purely random, thermally induced motion of *charge carriers*.

Note: According to the type of *charge carriers* undergoing diffusion, it is subdivided into electron diffusion, *hole* diffusion, *polaron* diffusion, *soliton* diffusion, *etc.* See also *electric drift*.

2.9 charge carrier generation
charge generation

Process whereby *charge carriers* are created [1].

Note 1: The charge carrier generation in the low-permittivity organic *semiconductors* usually proceeds in two steps: (i) formation of an *exciton*, and (ii) the *exciton dissociation* to mobile *charge carriers*.

Note 2: The energy needed for the charge carrier generation can be gained from photon absorption (photogeneration), from thermal motion of *lattice* atoms (thermal generation), from an electric field discharge or from another charge carrier with sufficiently high kinetic energy *(impact ionization)*.

2.10 charge carrier injection

Process whereby *charge carriers* in excess of the thermodynamic equilibrium level are introduced into a *conductor*, a *semiconductor* or an insulator from another material.

Note: See *double injection, electroinjection, photoinjection* and *thermal injection.*

2.11 charge carrier mobility, μ
charge mobility

Drift velocity (v_d) of *charge carriers* divided by the electric field strength (E).

$$\mu = v_\mathrm{d}/E \quad (\text{unit: m}^2\text{V}^{-1}\text{s}^{-1})$$

2.12 charge carrier recombination
charge recombination

Process whereby an electron in the *conduction band* (in LUMO level) loses its excess energy and re-occupies the energy state of a hole in the *valence band* (in HOMO level).

Note 1: In a thermally equilibrated material, generation and recombination of *charge carriers* are balanced yielding an equilibrium *charge carrier concentration* that is predictable from Fermi-Dirac statistics.

Note 2: Based on the mechanism of the charge carrier recombination we distinguish: Auger recombination, *geminate recombination, radiative charge carrier recombination, stimulated radiative charge carrier*

recombination, band-to-band recombination and localized-level-assisted (trap-assisted) recombination that dominate in organic *semiconductors*. See also *doping*.
Note 3: This new definition replaces the one given in reference [7].

2.13 charge density

Electric charge per unit dimension it occupies; *(i)* per unit length: linear charge density, *(ii)* per unit surface: surface charge density or *(iii)* per unit volume: volume charge density [11]; upgraded.

Note 1: The charge density can have a positive as well as negative value depending on the charge sign.
Note 2: Charge density should not be confused with the *charge carrier concentration*.

2.14 charge transfer (CT)

Transfer of *charge carriers* between two sites of the same molecular entity (intramolecular CT) or between two molecular entities occurring in close proximity (intermolecular CT).

Note 1: Electrons are implicitly considered as the *charge carriers* subject to a transfer. If other *charge carriers* (protons, *quasiparticles*) are considered, they should be explicitly mentioned.
Note 2: The molecular entity or the entity region from which electron(s) is(are) released is an electron donor while the molecular entity or the entity region accepting electron(s) is an electron acceptor.
Note 3: See also *charge transfer complex, charge transfer state, charge transfer transition*.

2.15 charge-transfer complex

CT complex

Complex whose electronic transition to the *excited state* is accompanied by a transfer of electronic charge between its constituents.

Note 1: The electrostatic attraction resulting from the charge transfer stabilizes the formed complex. Occurrence of the CT transition in a solution of the complex is solvent dependent.
Note 2: In coordination chemistry, CT complexes are classified according to the direction of the charge transfer to: metal-to-ligand (MLCT) and ligand-to-metal (LMCT) charge transfer complexes.
Note 3: A use of the term charge transfer complex for a geminate electron-hole pair, also called a CT pair, is discouraged.

2.16 charge-transfer exciton

Exciton formed by a *charge-transfer transition*.

2.17 charge-transfer state

CT state

State related to the *ground state* by a *charge-transfer transition* [9, 12].

2.18 charge-transfer transition

CT transition

Electronic transition in which a large fraction of electric charge is transferred from one region of a molecular entity, called the electron donor, to another, called the electron acceptor (intramolecular CT) or from one molecular entity to another (intermolecular CT) [9, 12].

2.19 chromophore

Part of a molecular entity, associated with electronic transition(s), responsible for a spectral band occurring at a wavelength above 200 nm [9]; modified.

Note 1: The term arose in the dyestuff industry, referring originally to the groupings in the molecule that are responsible for the dye's color. Nowadays, it is also concerned with bands in other spectral regions such as the near infrared.

2.20 conducting polymer see electrically conducting polymer (see also Note 1 in *conductivity*)

2.21 conduction band

Vacant or partially occupied set of many closely spaced electronic levels (*energy band*) in a lattice, in which electrons can move freely or nearly so [9, 12]; modified.

2.22 conductivity (general meaning)

Intensive quantity characterizing the ability of a material to transmit energy, or *charge carriers* [13].

Note 1: The entity transmitted such as electric charge, heat, light and sound, should be specified by the respective adjective electric (electronic, hole, ionic), thermal, optical or acoustic, *etc.*
Note 2: The obsolete term "specific conductance" should no longer be used.
Note 3: See also *electric conductivity*, *ionic conductivity*, *protonic conductivity* and *photoconductivity*.

2.23 conductor

Material having the ability to transmit energy or *charge carriers* or both [10].

Note: The nature of the conductor is specified by the entity transmitted, *e.g.*, electric (electron, hole, ion), thermal (heat) and acoustic.

2.24 conjugated polymer

A polymer composed of molecules whose backbone is a sequence of alternating single and multiple bonds:

$\left[\mathrm{CR^1{=}CR^2}\right]_n$	$\left[\mathrm{Ar{-}CR^1{=}CR^2}\right]_n$	$\left[\mathrm{Ar}\right]_n$	$\left[\mathrm{Ar{-}C{\equiv}C}\right]_n$
polyvinylenes	*polyarylenevinylenes*	*polyarylenes*	*polyaryleneethynylenes*

where R^1 and R^2 are each hydrogen, alkyl, aryl or heteroaryl and Ar is arenediyl (formerly: arylene) or heteroarenediyl (formerly: heteroarylene) [14]; modified.

Note 1: Overlaps of neighboring π-orbitals across intervening σ-bonds in a conjugated molecule results in *delocalization of π-electrons* along the molecule backbone. This effect which, however, is limited by *Peierls distortion* gives the *electric conductivity* to conjugated polymers.

Note 2: Conjugated polymers are mostly linear or branched polymers. However, they can also have a dendritic [15], hyperbranched [15], network [14, 16], rotaxane [17] or metallo-supramolecular [18] chain architecture [14].

Note 3: Polymers such as *polysilanes*, polygermanes and polystannanes with significantly occupied LUMO orbitals due to low *bandgap energy* and thus show the *delocalization of electrons* sometimes called σ-conjugated polymers [14].

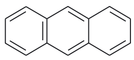
2.25 π-conjugated system

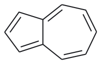
Molecule or a part of a molecule, of which structure may be represented as a system of alternating single and multiple bonds, in which, eventually, a multiple bond can be replaced by an atom with a pair of non-bonding electrons or an atom carrying a negative charge [19]; modified.

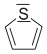
Note 1: Examples of conjugated systems are *conjugated polymers* and molecule species whose formulas drawn in terms of the *valence bond theory* are as follows:

$CH_2{=}CH{-}CH{=}CH_2$
buta-1,3-diene

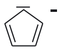
$CH_2{=}CH{-}CH{=}O$
propenal


anthracene


azulene



thiophene



cyclopentadienyl anion

Note 2: Alternating arrangement of the single and multiple bonds allows the *delocalization of electrons*, which stabilizes conjugated systems. The most effective stabilization show planary cyclic systems with $2n + 2$ delocalized electrons (where n is integer), so-called aromatic systems. The last two examples above are the species where the pair non-bonding electrons (thiophene) or electrons of negatively charged atom are delocalized together with π-electrons giving an aromatic system.

Note 3: Due to the *delocalization of electrons* a formula drawn in terms of the *valence bond theory* does not fully describe the structure of a conjugated species, which actually is a combination of two or more limiting or intermediate resonance structures that are in a dynamic equilibrium. The *molecular orbital theory* which directly provides extended molecular orbitals spread over all contributing atoms allows better understanding of the electronic and optical properties of a conjugated system.

2.26 conjugation of chemical bonds

conjugation

Interconnection of a series of formally localized adjacent orbitals leading to efficient *delocalization of electrons* over all involved chemical bonds and atoms [12]; modified.

Note 1: Interconnection of formally localized orbitals follows directly from the *molecular orbital theory*.

Note 2: The term *π*-conjugation refers to systems where electrons are delocalized due to overlaps of π-orbitals of vicinal (bonded to two adjacent atoms) multiple bonds across intervening σ-bond(s).

Note 3: The term σ-conjugation refers to the systems without multiple bonds, such as *polysilanes*, where electrons are delocalized over geminal (bonded to the same atom) σ-orbitals.

Note 4: The size of a π-*conjugated system* is sometimes characterized by a quantity called "conjugation length" defined as the number of specified units (usually multiple bonds or conjugated rings) forming the *conjugated system*. However, the real (effective) *extent of electron delocalization* in such systems is mostly lower than the system size owing to *Peierls distortion* and structural defects.

2.27 Coulomb radius

Distance between two oppositely charged *charge carriers* at which the energy of their Coulombic attraction is equal to kT, where k is the Boltzmann constant and T the absolute temperature.

Note: See also *charge carrier recombination*.

2.28 dark electric conductivity

dark conductivity

Electric conductivity of a material in the dark where the *free charge-carrier photogeneration* is excluded.

Note: The dark electric conductivity of a material in thermal equilibrium is proportional to the product of the *concentration of free charge carriers* and the *charge carrier mobility*. See also *photoconductivity*.

2.29 degenerate orbitals

Orbitals whose energy levels are equal in the absence but unequal in the presence of an external field [19].

Note: The degeneracy can be removed by an external electric or magnetic field.

2.30 delayed luminescence

Luminescence decaying more slowly than that expected from the rate of decay of the emitting state [9].

Note: According to Jablonski diagram, the delay is related to the existence of metastable or triplet states with energies lower than excited singlet state. Back reactions can lead to repopulation of the first excited singlet state, whose decay gives rise to the delayed luminescence.

2.31 delocalization of electrons

Redistribution of electron density in a molecular entity as compared with a model assuming individual atoms in the same valence states connected by localized bonds [19, 20]; modified.

Note 1: Topological modes of the electron delocalization include:

a) ribbon (one-dimensional) delocalization of π- or σ-electrons or both, which is typical of linear *conjugated polymers* that are therefore termed one-dimensional *conductors*;
b) surface delocalization of π- or σ-electrons or both through an overlap of radially oriented orbitals of a cyclic molecule such as a molecule of cyclopropane or benzene;
c) volume delocalization of σ-electrons through an overlap of σ-orbitals directed inside a molecular polyhedron, *e.g.*, in tetrahedrane or carboranes.

Note 2: A delocalized electron is not associated with a particular atom or particular covalent bond but occupies an extended orbital spread over several to many atoms or the whole *lattice*.
Note 3: Extensive delocalization of electrons is typical of metals, *semiconductors*, graphite, *conjugated polymers*, *polysilanes*, boranes, conjugated compounds such as organic dyes and others.
Note 4: See also conjugation, *extent of electron delocalization,* and *molecular orbital theory*.

2.32 **density of energy states** (in solid state physics)

density of states

Number of energy states within an energy interval divided by volume and that energy interval [11].

Note: Density of electronic energy states is not uniform within an *energy band*; in general, it is the highest in the middle of the band and approaches zero at the band boundaries (top and bottom of the band).

2.33 **Dexter excitation transfer**

electron exchange excitation transfer

Excitation transfer by the electron exchange mechanism, which is possible only in a system with overlapping wave functions of the energy donor and acceptor [7]; (shortened).

Note: This mechanism is dominant in the triplet-triplet energy transfer.

2.34 **dielectric material**

dielectric

Material which polarizes when exposed to an external electric field, because it creates its own internal electric field oriented against the external field [1, 10].

Note 1: Dielectrics are divided into polar and nonpolar. The polar ones contain dipolar groups and their *poling* (polarization process) consists in the orientation of these dipoles by an external electric field. It is the so-called orientation polarization, which can but may not be complete due to competitive thermal motion. *Poling* of some polar dielectrics such as *fluoropolymers* gives materials with a stabilized polarized structure known as *electrets*. *Poling* of a non-polar *dielectric* is always temporary since it consists in displacements of electrons (electronic polarization) or ions in crystals (ionic polarization) giving induced dipoles that decay immediately after the removal of the field.
Note 2: Dielectrics are key materials for the construction of capacitors.
Note 3: See also *ferroelectric polymer*, *polarizability* and, *polarization density*.

2.35 **diffusion current** (in solid-state physics)

Current caused by diffusion of *charge carriers* due to their concentration gradient.

2.36 **dispersive transport** (of charge carriers)

Irregular charge transport in which *charge carriers* move with an ill-defined mean velocity owing to the high variety of dwell times spent at different transport sites.

Note: See also *hopping transport*.

2.37 **dopant** (in electronics)

doping agent

Chemical agent or additive used to generate free *charge carriers* or to increase their thermal-equilibrium concentration in a parent material.

Note 1: Typical dopants to organic polymers (compounds) are:

a) oxidants which generate or increase the concentration of free *holes*;
b) reductants which generate or increase the concentration of free *electrons*;
c) strong Brønsted acids which give to a polymer or increase its *protonic conductivity*.

Note 2: See also *conjugated polymers, doping, proton doping, polyanilines* or *polybenzimidazoles*.
Note 3: This new definition replaces the one given in reference [21].

2.38 **doping** (in electronics)

Chemical or electrochemical modification of a parent material giving a new structurally similar material with an enhanced *electric conductivity* or efficiency of the free *charge carrier generation* or both.

Note 1: Doping can be performed by a *dopant* or by an electrode reaction (*redox doping*).
Note 2: Doping of an insulating material determines the *conductivity* type (electronic, *hole*, protonic, ionic, polaronic) of the resulting semiconducting or conducting material.
Note 3: Oxidation doping is called p-doping since it gives conductors of positive *charge carriers* (*holes* or positive *polarons*). Reduction doping is called n-doping since it gives conductors of negative *charge carriers* (electrons or negative *polarons*). Doping by Brønsted acids is called *proton doping*.
Note 4: This definition replaces that published in ref. [21].

2.39 **double injection**

double charge carrier injection

Simultaneous injection of both types of *charge carriers* (electrons and *holes*) into a material or a device.

Note: Double injection is used in production of *electrets* and function of *light-emitting diodes*.

2.40 **drift** (in general)

General term used for an oriented motion of otherwise randomly moving objects or an oriented change of otherwise randomly fluctuating parameter, which is induced by an external force field.

Note 1: Examples of drifts are *electric drift* characterized by the *drift current* and *drift velocity*, genetic drift – evolution changing characteristics of organisms over time, and instrumentation drift – a slow long-term oriented change of some parameters of a device.
Note 2: This new definition replaces the one given in ref. [22] considering only instrumentation drift.

2.41 **drift current,** i_d

Electric current caused by *electric drift*.

Note: See also *charge carrier diffusion, diffusion current, drift*.

2.42 drift velocity (in electricity), v_d

Average velocity that a *charge carrier* attains due to an applied electric field.

Note 1: If an electric field is absent, *charge carriers* move randomly. An applied electric field induces *drift* (net movement) of *charge carriers* in a preferred direction. Average net velocity of this movement is called the drift velocity v_d.

Note 2: The drift velocity of a *charge carrier* is directly proportional to the applied electric field strength E:

$$v_\mathrm{d} = \mu E$$

where constant μ is the *charge carrier mobility* in the given material.

2.43 electret

Dielectric material with a permanent or quasi-permanent electric dipole.

Note 1: A real-charge electret is obtained by the *charge carrier injection* onto the surface or into a parent *dielectric material*. It may contain either positive or negative excess charges or both, which must be trapped so that a good insulating parent *dielectric material* such as a fluoropolymer must be used.

Note 2: An oriented-dipole electret is obtained by *poling* a parent *dielectric material* with dipolar groups at a temperature above the glass transition temperature T_g, and eventual next stabilization of the structure by cooling the electret down below T_g or by crosslinking.

Note 3: Electrets are electric equivalents of magnets; **electr**ic magn**ets**. Some oriented-dipole electrets are *ferroelectric polymers* and *piezoelectric polymers*. Quartz is an example of the natural electret.

2.44 electric conductivity

Reciprocal of electric resistivity [11, 13, 20] modified.

Note 1: Specific quantity characterizing the capacity of a material to conduct electric current, unit S m^{-1}.

Note 2: The obsolete term “specific electric conductance” should no longer be used.

Note 3: See also *dark electric conductivity, ionic conductivity* and *photoconductivity.*

2.45 electric conductor

Material that is able to transmit electric current.

Note: See also: *electrically conducting polymer, semiconductor.*

2.46 electric drift

Oriented flow of otherwise randomly moving *charge carriers* induced by an applied external electric field.

2.47 electrically conducting polymer

intrinsically conducting polymer
conducting polymer

Polymeric material that exhibits bulk *electric conductivity* [23].

Note 1: A conducting polymer can be an *intrinsic (semi)conductor*, when conduct current by itself, or an *extrinsic (semi)conductor* whose conductivity is in prevail a result of *doping*.
Note 2: A polymer showing a substantial increase in *electric conductivity* upon irradiation with ultraviolet or visible light is a *photoconducting polymer*; an example is *poly(N-vinylcarbazole)*.
Note 3: A polymer that shows electric *conductivity* due to the transport of ionic species is called an *ion-conducting polymer;* an example is sulfonated *polyaniline*. When the transported ionic species is a proton as, *e.g.*, in the case of fuel cells, it is called a proton-conducting polymer.
Note 5: See also *conductivity, photoconductivity* and *electrically conducting polymer composite*.

2.48 electrically conducting polymer composite

conducting polymer composite

Composite composed of a non-conducting polymer matrix in which irregular powdered or fibrous particles of an electrically conducting material are evenly dispersed in an amount exceeding the *percolation threshold* for *electric conductivity* and so the composite exhibits *electric conductivity* close to that of the conducting filler.

Note 1: Conventional rubbery polymers are mostly used as the insulating matrix and powdered metals or carbon black as the dispersed phase in commercialized conducting polymer composites [1, 11].
Note 2: Conducting polymer composites are extrinsically conducting polymeric materials since the matrix does not act as an *electric conductor* but only as a container for the active *electric conductor*.

2.49 electrochemiluminescence

electrogenerated chemiluminescence

Luminescence produced by an electrochemical reaction [7]; modified.

Note 1: Electrochemiluminescence should not be confused with *electroluminescence* where no chemical reaction is involved.
Note 2: This definition replaces the definition given in refs [7, 20], where *electroluminescence* is given as a synonym for electrochemiluminescence.

2.50 electrochromic effect

electrochromism

Reversible change in the material color or opacity in response to or a change in the applied electric field.

Note 1: Electrochromism is an *electro-optic effect* that consists in reversible switching between two or more redox states with different optical spectra in response to the applied outer electric field.
Note 2: This definition replaces that one in ref. [7] which identifies electrochromism with the Stark effect.

2.51 electrochromic polymer

Polymer that exhibits *electrochromism*.

2.52 electrofluorescence

Electroluminescence originated from singlet-state *excitons*.

2.53 electroinjection

Process of *charge carrier injection* induced by an applied external electric field.

2.54 electroluminescence

Luminescence in response to an electric current passed or passing through a luminescent material.

Note 1: Electroluminescence is an optoelectric phenomenon that is caused by *radiative recombination* of mobile *electrons* and *holes* injected into a luminescent material by *double injection*.

Note 2: Electroluminescence generated from singlet *excitons* is referred to as *electrofluorescence*, while that generated from triplet-state *excitons* is *electrophosphorescence*.

Note 3: Electroluminescence should not be confused with a radiation emitted by an electrically heated body or with *electrochemiluminescence*, which is induced by an electrochemical reaction.

Note 4: This definition replaces the definition given in refs [7, 20], where electroluminescence is given as a synonym for *electrochemiluminescence*.

2.55 electroluminescent polymer

Polymer that shows *electroluminescence*.

2.56 electromagnetic field

Physical field composed of two interconnected, mutually orthogonal fields, an electric field and a magnetic field, which mediates interactions of charged, dipolar and multipolar objects.

Note: The electromagnetic field produced by one charged or polar object affects other charged or polar objects, which is the essence of electromagnetic interaction – one of the four basic forces in nature.

2.57 electromagnetic field responsive polymer

Polymer showing a noticeable response of its physical or chemical properties during or upon exposure to an *electromagnetic field* or one of its components: electric field and magnetic field.

2.58 electron affinity

Energy released when a free electron is attached to a neutral atom or molecule [11, 20].

Note: See also *work function*.

2.59 electron-deficient molecule

Molecule that has fewer valence electrons than required for forming normal two-center two-electron chemical bonds and thus contains multicenter chemical bonds.

Note 1: Binding of atoms into molecules, clusters and macroscopic bodies in electron-deficient compounds is mediated by *delocalized electrons*, each being shared by three or more atoms.
Note 2: Metals are typical electron-deficient compounds in which extreme *delocalization of electrons* across the whole macroscopic body exists.
Note 3: Boron, boranes, carboranes and related compounds are typical compounds with electron-deficient molecules in which boron and some other atoms are bound by multicenter two-electron bonds, such as by the two-electron three-center bond in which two electrons bind three atoms.
Note 4: See also *conjugation, electron-rich molecule, extent of electron delocalization.*

2.60 electron-rich molecule

Molecule that has more valence electrons than is needed to link its atoms by single covalent bonds.

Note 1: Molecules of unsaturated hydrocarbons or aromatic and heteroaromatic compounds are typical electron-rich molecules. Such compounds can be called electron-rich compounds.
Note 2: Formally excess electrons present in a molecule containing conjugated multiple bonds are *delocalized electrons*. Non-bonding valence electrons present in molecules with heteroatoms, such non-bonding electrons of nitrogen, phosphorus and sulfur atoms, are also taken into account.

2.61 electron transfer (ET)

Transfer of an electron from one molecular entity to another, or between two localized sites in the same molecular entity [12].

Note 1: ET is a redox process, since the oxidation state of both reacting sites is changed in this process. The site (entity) releasing an electron is called the electron donor center or reducing center, the site (entity) accepting an electron is called the electron acceptor center or oxidation center.
Note 2: Outer-sphere electron transfer is an ET during which two participating redox centers are not linked via any bridge and so the electron hops through space from the donor to the acceptor center. This ET is by definition an intermolecular electron transfer.
Note 3: Inner-sphere electron transfer is an ET during which two participating redox centers are covalently linked. This transfer can be an intramolecular electron transfer if covalent linking of redox centers is permanent or an intermolecular electron transfer if the covalent linking is only temporary.
Note 4: The ET in which participating redox centers are located in different phases is referred to as heterogeneous electron transfer or inter-phase electron transfer.

2.62 electron tunneling

electron quantum tunneling

Quantum mechanical effect of passing an electron through a potential energy barrier separating two energy equivalent regions [1, 10].

Note: The electron tunneling effect is exploited, *e.g.*, in scanning tunneling microscopes, pressure sensors based on *quantum tunneling polymer composites* and in touchable panels of electronic devices.

2.63 electro-optic effect

Change in the optical properties of a material in response to a change in an external electric field strength.

Note 1: Changes in the absorption coefficient, color, refractive index, permittivity or optical activity of a material are typical examples of electro-optic effects. See also *electrochromism*.

Note 2: Electro-optic is not a synonym for *optoelectronic*.

2.64 electrophosphorescence

Electroluminescence originated from triplet-state *excitons*.

2.65 electrorheological effect

Reversible change in the apparent viscosity of a liquid system such as suspension of polar or good polarizable microparticles in an oil, upon exposure of an electric field.

Note: Interaction of electric dipoles induced on suspended particles produces strands of particles spanning between electrodes, which results in a giant increase in the viscosity of the suspension (up to 5 orders of magnitude) during its exposure to an electric field.

2.66 energy band

electronic band

Quasi-continuous range of discrete energy levels that an electron is either allowed (an occupied band) or forbidden (forbidden band or band gap) to occupy in a molecule or solid.

Note 2: See also *bandgap energy*, and *energy band theory* and *energy gap*.

2.67 energy band theory

electronic band theory

Theory describing the electronic structure of a solid in terms of energy intervals, called energy bands that are allowed or forbidden for occupation by electrons.

Note 1: The energy band theory stems from the solution of the Schrödinger equation for electron waves moving in a periodic crystal *lattice* where, due to the wave diffractions, only some directions of the wave propagation characterized by the wave vector (so-called *k*-vector) are allowed.

Note 2: When several atoms form a molecule, their atomic orbitals are transformed into a set of discrete bonding and antibonding molecular orbitals (energy levels), the number of which is proportional to the number of involved atoms. The energy levels that an electron is allowed to occupy are separated by energy intervals without any energy levels that an electron can occupy. If many atoms are linked together to form a *lattice*, the number of energy levels that the electrons are allowed to occupy becomes exceedingly large. Among these energy levels, large subsets of energy levels exist in which energy differences between individual levels are so small that they may be regarded as a quasi-continuum (individual energy levels are of no importance). The subset of energy levels that can be occupied by electrons is named allowed energy bands. The allowed bands are separated by energy intervals that electrons cannot occupy, which are called forbidden bands or energy bandgaps.

2.68 energy gap
bandgap

Energy interval in a *lattice* where no electronic state exists.

2.69 excimer

Electronically excited dimeric complex formed from one excited and one ground-state molecular entity, which decays immediately after deexcitation since does not exist in the ground state [7, 10], modified.

Note 1: The term excimer is derived by abbreviating the term excited dimer and in a narrow sense refers to excited dimers of the same molecular entities (homoexcimer). An excimer composed of different molecular entities (heteroexcimer) is usually referred to as an *exciplex*.

Note 2: Compared to the free parent molecules, the excimer absorption as well as emission is red-shifted. Excimer emission often occurs in bulk organic luminescent materials where the excimer is readily formed due to the low conformational freedom of molecules.

2.70 exciplex

Excimer composed of different molecular entities, *i.e.*, hetero-excimer.

2.71 **excitation** (in physics and chemistry)

Transition of a system from one state to another of higher energy [20, 24].

Note 1: Mostly transition from the system *ground state* into an *excited state* is considered if the initial state is not specified.

Note 2: Electronic, vibrational and rotational excitations of molecular entities are generally considered in chemistry and molecular physics. These excitations are not independent but linked. Linking of electronic and vibrational states, so-called vibronic coupling, connects electronic and vibrational excitation into vibronic excitation. Similarly, simultaneous electronic, vibrational and rotational excitation is referred to as a rovibronic excitation.

Note 3: The term excitation is sometimes incorrectly used as a synonym for a relatively long-living *excited state* of a multi-body system instead of the term *exciton*.

2.72 excited state

Any quantum state of a system in which the system energy exceeds its *ground state* energy ([7] corrected).

Note: This term refers to electronic, vibrational and rotational *excitations* of molecular entities as well as various types of *excitations* in *lattices* or metal nanoparticles.

2.73 exciton

Quasiparticle consisting of an electrostatically bound (correlated) *electron-hole* pair [7]; shortened.

Note 1: Exciton is a fundamental electrically neutral quantum of electronic excitation in condensed matter that can move in it like a particle transferring the energy but not a charge.

Note 2: There are two basic types of excitons:

a) weakly bound (Mott-Wannier) excitons (binding energy up to ca 0.5 eV) whose radii exceed the *lattice* spacing, which are typical of inorganic semiconductors with medium-to-high relative permittivity (high electrostatic shielding) and small *bandgaps;*
b) strongly bound (Frenkel) excitons (higher binding energy) with radii comparable to the *lattice* spacing, which occur in the low relative permittivity materials (low electrostatic shielding, *i.e.*, high Coulomb attraction), such as in most of organic materials.

Note 3: See also *charge transfer exciton, exciton annihilation, exciton dissociation* and *exciton-phonon coupling.*

2.74 exciton annihilation

Interaction of two *excitons* resulting in their decay and radiative emission of the stored excitation energy.

2.75 exciton diffusion

Random movement of an *exciton* from one molecular entity to another or from one part of a molecular entity or a *lattice* to another part of the same kind.

2.76 exciton dissociation

Fission of an *exciton* into independent, Coulombically unbound mobile *charge carriers*: an electron and a *hole*, or a negative and a positive *polaron*.

2.77 exciton mean free path

exciton mean pathway

Mean distance that an *exciton* travels from the site of its creation to the site where it radiatively or non-radiatively decays or dissociates into *charge carriers*.

2.78 exciton-phonon coupling

Interaction in which a part of the *exciton* energy is converted into the *lattice* vibrational energy and vice versa.

2.79 extent of electron delocalization

effective conjugation length

Magnitude of the region in a molecule over which a molecular orbital occupied with *delocalized electrons* is extended.

Note 1: In a small molecule, the extent of electron delocalization is usually quantified by the number of delocalized electrons included in the extended orbital or by the number of bonds or atoms or both over which the extended molecular orbital is spread.

Note 2: In a larger molecule or macromolecule, delocalized electrons are mostly divided over several to many extended orbitals of various magnitudes separated by orbitals where electrons are practically localized. Therefore, the average number of delocalized electrons per one extended orbital, or the average number of bonds or atoms or both over which a mean extended orbital is spread, are used as a measure of the extent of the electron delocalization. See also *Peierls distortion.*

Note 3: The extent of electron delocalization in a conjugated molecule is often termed effective *conjugation* length or effective extent of *conjugation.*

2.80 external quantum yield

Quantum yield relating to the whole device or the overall process involved.

Note: See also *internal quantum yield*.

2.81 extrinsic semiconductor

Semiconductor whose electric properties are largely determined by the *dopant* “impurities” present.

Note 1: Phosphorus-doped silicon, *i.e.*, silicon, in which some Si atoms are replaced with phosphorus atoms, or iodine doped *poly(acetylene)* are examples of extrinsic semiconductors.

Note 2: See also *intrinsic semiconductor* and *charge carrier generation*.

2.82 Fermi energy, E_F

Energy difference between the highest and the lowest occupied energy states in a system of non-interacting fermions at the zero absolute temperature [1, 10].

Note: The Fermi energy can be also defined as the energy of the highest occupied energy state in a system of fermions at absolute zero temperature if the ground state energy is equal to zero.

2.83 Fermi level

Equilibrium electronic energy level in a solid for which the probability of being occupied is equal to ½ [10].

Note 1: Fermi level of energy μ appears in the Fermi-Dirac distribution function $f(\varepsilon)$ of electron energies ε:

$$f(\epsilon) = \frac{1}{1 + \exp \frac{\epsilon - \mu}{kT}}$$

where $f(\varepsilon)$ is the probability that an electron occurs on the energy level with energy ε, k is the Boltzmann constant and T is the absolute temperature.

Note 2: Fermi level of a solid is in fact the average work required to add an electron to the solid. Hence it corresponds to the chemical potential of electrons in a solid.

Note 3: Fermi level is a function of temperature, just like any other chemical potential. Therefore, it must not be confused with *Fermi energy* that is defined for zero absolute temperature.

2.84 ferroelectric polymer

Polymer that exhibits permanent *dielectric polarization* that can be changed or reversed by applying an external electric field [23]; modified.

Note 1: Spontaneous *polarization* of a *dielectric* polymer occurs if a parallel alignment of electric dipoles present in the polymer provides a structure that is thermodynamically stable in the absence of the external electric field. If this structure can be converted to another stable one by an electric field of the opposite direction, the *polarization* vs. electric field strength curve exhibits a hysteresis like the magnetic polarization curve of a *ferromagnetic polymer* (material). Hence this behavior is termed ferroelectric behavior, this material property is called ferroelectricity and materials showing this behavior are referred to as ferroelectric materials or, in short, ferroelectrics.

Note 2: Switching a ferroelectric polymer between two states is utilized in ferroelectric memories and capacitors. *Fluoropolymers* such as poly(1,1-difluoroethylene), poly(1,1,2-trifluoroethylene) and poly(1-fluoroethylene) are typical examples of ferroelectric polymers.

Note 3: Ferroelectric polymers are oriented-dipole *electrets* that show piezoelectricity and pyroelectricity, which makes them useful for sensor applications. See also *piezoelectric polymer*.

2.85 **ferromagnetic polymer**

Polymer that exhibits magnetic properties because it has unpaired electron spins aligned parallel to each other or electron spins that can easily be so aligned [23].

Note: See also *ferroelectric polymer*.

2.86 **field-effect transistor** (FET)

Transistor in which the flow of *charge carriers* from source to drain is controlled by the potential applied to the gate [1].

2.87 **fill factor** (of a solar cell), f_{FF}

Ratio of the real maximum output power, $P_{\max}$, that can be obtained with an actual *solar cell* to the product of the open-circuit potential, V_{oc}, and short-circuit photocurrent, I_{sc} [1]:

$$f_{\mathrm{FF}} = P_{\max}/V_{\mathrm{oc}}I_{\mathrm{sc}}$$

Note 1: The $P_{\max}$ value is obtained from the cell volt-ampere characteristic as the maximum of the product $V{\cdot}I = P$. Note that the product $V_{\mathrm{oc}}{\cdot}I_{\mathrm{sc}}$ is not a theoretical maximum output power of the cell, since the product is zero at both these values as $I = 0$ for the open circuit and $V = 0$ for short circuit.

2.88 **Förster resonance energy transfer** (FRET)

Förster excitation transfer
dipole-dipole excitation transfer

Non-radiative excitation transfer between two molecular entities separated by a distance considerably exceeding the sum of their van der Waals radii [9].

Note 1: FRET is described in terms of the weak dipole-dipole coupling. The FRET rate constant, k_{T}, is inversely proportional to the sixth power of the donor-acceptor distance, r:

$$k_{\mathrm{T}} = k_{\mathrm{D}}\,(R_0/r)^6$$

where k_{D} is the rate constant of the excited donor decay and R_0 is the distance at which the transfer and spontaneous decay of the excited donor are equally probable ($k_{\mathrm{T}} = k_{\mathrm{D}}$).

Note 2: Due to its extreme sensitivity to small changes in the donor-acceptor distance, FRET is often used to determine the nanometer scale distances between two *chromophores* (fluorophores).

2.89 free charge-carrier photogeneration

charge-carrier photogeneration

Generation of free *charge carriers* by photons.

2.90 geminate recombination (of charge carriers)

Recombination of the same electron and *hole* that formed together in the same *charge carrier generation* event [12]; adapted.

Note: The energy released in this recombination is mostly transformed to *lattice* vibrations (*phonons*).

2.91 ground state

ground energy state

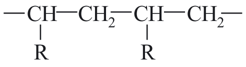
State with the lowest Gibbs energy of a system [12].

2.92 head-tail isomerism

HT-isomerism
regioisomerism

Constitutional isomerism of polymeric (oligomeric) chains composed of identical non symmetric repeating units consisting in different orientations of the units.

Note 1: In the repeating unit of a vinyl polymer: $-CHR-CH_2-$, the substituent-bearing group CHR is denoted “head” (H) while the other one “tail” (T). There exist three modes how two such units can be linked in a chain: head-to-tail (HT), head-to-head (HH) and tail-to-tail (TT).

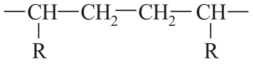


$-\underset{R}{\underset{|}{CH}}-CH_2-\underset{R}{\underset{|}{CH}}-CH_2-$

head-to-tail (HT) linking

$-CH_2-\underset{R}{\underset{|}{CH}}-\underset{R}{\underset{|}{CH}}-CH_2-$

head-to-head (HH) linking



$-\underset{R}{\underset{|}{CH}}-CH_2-CH_2-\underset{R}{\underset{|}{CH}}-$

tail-to-tail (TT) linking

Note 2: The uniformity/non-uniformity of repeating units’ orientation determines the regularity/irregularity of macromolecules. See also *regular polymer, regioregular polymer, regioirregular polymer.*

2.93 heterojunction

Interface between dissimilar crystalline or amorphous solid phases that have unequal *bandgap* levels.

Note 1: Heterojunction allows efficient dissociation of *charge carriers,* which is utilized, *e.g.,* in diode lasers, heterojunction bipolar transistors and high electron *mobility* transistors.

Note 2: See also *homojunction.*

2.94 highest occupied molecular orbital (HOMO)

Highest energy molecular orbital that is at least partly occupied in a ground state molecular entity [12].

Note: See also *lowest unoccupied molecular orbital, molecular orbital theory.*

2.95 hole

electron hole

Quasiparticle, a conceptual *charge carrier* opposite to electron, defined as the absence of electron at a position where it should be present if a *lattice* is in its ground state (valence band normally filled).

Note 1: An electron hole is a conceptual (mathematical) opposite of an electron, while a positron is the antimatter analog of an electron.
Note 2: In condensed matter, a hole is created if an electron originally occurring in the *valence band* is excited into *conduction band* thus leaving a positively charged site in its previous position.
Note 3: The hole has a positive electric charge (+e, where e is an elementary charge) and also an effective mass which, in most *semiconductors* is higher than the mass of the electron.

2.96 hole-transporting material

Material, typically a *semiconductor*, in which *holes* are predominant mobile *charge carriers*.

2.97 homojunction

pn-junction

Interface occurring between two similar *semiconductors* with equal *bandgaps*.

Note 1: Homojunction mostly occurs at the interface between n-doped and p-doped *semiconductor* of the same nature, typically silicon. This type of homojunction is currently called a *pn junction*.
Note 2: See also *heterojunction*.

2.98 hopping transport

Incoherent transport of *charge carriers* by hopping between adjacent energetically nearly equivalent localized sites [9, 12]; modified.

Note 1: Hopping transport is typical of molecular solids and polycrystalline and amorphous semiconductors. It takes place via *electron tunneling* or by overcoming energy barriers (typical of ions), and is the opposite of intra-molecular transport (band transport) of charge carriers in metallic conductors.
Note 2: A hopping *charge carrier* spends most of time sitting idle on a localized site and then hops (tunnel) to an adjacent site. As a result, the *charge carrier mobility* at hopping transport is low (typically below 0.01 cm^2/Vs) and is an increasing function of temperature. See also *dispersive transport*.

2.99 hot electron

Electron that is out of the thermal equilibrium with its environment and has enough kinetic energy to overcome potential barriers to travel between different regions of a molecule or *lattice* [1].

2.100 hyperfine interaction

Interaction between the electron spin and the nuclear spin [9].

2.101 **impact ionization** (in a semiconductor)

Charge carrier generation by another *charge carrier* possessing a high kinetic energy, which knocks an electron out of the *HOMO* into the *LUMO* or still higher state so creating a new electron–*hole* pair.

2.102 internal quantum yield

Quantum yield relating to a single component or a part of a device or a partial step of an overall process.

2.103 intrinsic semiconductor

Semiconductor in which mobile *charge carriers* are generated solely by thermal excitation of electrons.

Note 1: Intrinsic semiconductor is free of *dopants*, so that it has no energy states in the *bandgap*.

Note 2: Pure *conjugated polymers* such as *poly(ethene-1,2-diyl)* or *poly(pyrrole-2,5-diyl)* and other polymers with delocalized valence electrons such as *polysilanes* are examples of intrinsic semiconductors.

Note 3: See also *charge carrier generation*, *doping*, and *extrinsic semiconductor*.

2.104 ion-conducting polymer

Conducting polymer in which ionic species are mobile *charge carriers*.

Note: Protons are typical charge carriers in ion-conducting polymers. Such polymers are currently referred to as proton-conducting polymers. Examples are *polyanilines*.

2.105 ionic conductivity

Electric conductivity mediated by the transport of ions.

2.106 irregular polymer

Polymer composed of macromolecules whose structure essentially comprises the repetition of more than one type of constitutional unit, or macromolecules in which not all constitutional units are connected identically with respect to a directional sense [25].

Note: See also *head-tail isomerism*, *regular polymer* and *regioirregular polymer*.

2.107 **lattice** (in condensed matter physics)

Periodic grid-like ideal structure consisting of regularly arranged elementary repeating units.

Note 1: In the condensed matter physics, lattice models are currently used for modeling and theoretical studying of electric, magnetic and optical phenomena as well as materials properties. 1-Dimensional (1-D) lattice is used for modeling linear objects such as linear *conjugated* *polymer*s (see *Peierls distortion*), 2-D and 3-D lattices for modeling planar and spatial objects, respectively.

Note 2: Crystal (Bravais) lattices are the most famous examples of physical 3-D lattice models.

2.108 **light emitting diode** (LED)

Transducer–type device that converts an electric current into *luminescence* light.

Note: See also *electroluminescence*.

2.109 **lowest unoccupied molecular orbital** (LUMO)

Lowest-energy molecular orbital that is unoccupied in the *ground state* but occupied by one or more electrons if the molecular entity occurs in its first electronically excited state.

Note: See also *highest occupied molecular orbital, energy band theory* and *molecular orbital theory*.

2.110 **luminescence**

Spontaneous emission of radiation from an electronically and vibrationally (vibronically) excited species that is not in thermal equilibrium with its environment [7, 12].

2.111 **luminescent material (polymer)**

Material (polymer) that exhibits a *luminescence* [23].

Note: Luminescent is in general a material, in which *radiative charge carrier recombination* represents a significant mode of the overall *charge carrier recombination*.

2.112 **magnetoresistance**

Change in the electric resistance of a material in response to an external magnetic field.

2.113 **memristor**

memristive system

Electric component that can be reversibly switched between stable low- and high-resistive states.

Note: The term memristor is derived from the phrase memory resistor.

2.114 **mobility** (in general)

Drift velocity divided by the strength of the field causing the *drift* [20]; and [11].

Note: See also *charge carrier mobility, electrical drift*, and *drift current*.

2.115 molecular orbital theory

MO theory

Theory of quantum mechanics in which electrons in a molecule (*lattice*) are not assigned to particular bonds between atoms but move under the influence of all atoms.

Note 1: Within the MO theory, the wave function of *i*-th MO, ϕ_i, is expressed as a weighted sum of all atomic orbitals, χ_r (method known as the linear combination of atomic orbitals, LCAO):

$$\varphi_i = \sum_{r=1}^{N} c_{ri}\chi_r$$

where the coefficient c_{ri} is the contribution of the *r*-th atomic orbital to the *i*-th MO.

Note 2: MO theory is a counterpart of the *valence bond theory* in which electrons are assigned to individual bonds. MO theory fits perfectly for systems with delocalized electrons.

2.116 molecular switch

Molecule that can be reversibly switched between two or more stable states in response to a change in, *e.g.*, its microenvironment (pH, the presence of a ligand, temperature *etc.*), illumination or electric current.

Note 1: Molecules undergoing photoinduced reversible cis-trans isomerization or switching between redox state or protonation states (pH indicators) are examples of molecular switches.

2.117 nonlinear optical effect

Effect arising from a nonlinear dependence of the *polarization density*, *P*, on the electric field strength, *E*.

Note 1: For an optically linear (isotropic) material, $\boldsymbol{P} = \varepsilon_0\chi^{(1)}\boldsymbol{E}$ where $\chi^{(1)} = \varepsilon_\mathrm{r} - 1$ is the linear dielectric susceptibility, ε_r relative permittivity and ε_0 permittivity of vacuum. For an optically nonlinear material the dependence of **P** on **E** is extended about nonlinear terms. The linear term is responsible for normal optical phenomena connected with the light refraction and absorption. The quadratic term can be understood so that the refractive index depends on the electric field strength and the cubic term so that it depends on the light intensity. See also refs [9–11].

Note 2: Generation of the light with doubled or tripled frequency (frequency doubling or tripling), two-photon absorption, Raman scattering amplification and self-focusing effects are examples of nonlinear optical phenomena. High values of *E* are typically needed for a nonlinear optical phenomenon to be seen.

2.118 occupied band

Energy band occupied by electrons, typically the *valence band*.

2.119 ohmic contact

Electric junction which exhibits linear and symmetric current-potential dependence.

Note: The current is not rectified at an ohmic contact unlike the case of a *Schottky barrier*.

2.120 optically-active polymer

Polymer capable of rotating the polarization plane of a transmitted beam of linear-polarized light [23].

Note: The optical activity of a polymer originates from the presence of chiral elements such as chiral centers or chiral axes (helicity).

2.121 optically nonlinear polymer

Polymer that exhibits a *nonlinear optical effect* [23]; shortened.

2.122 optoelectronics

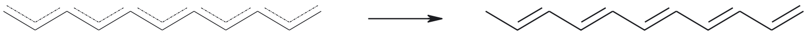
Branch of physics that deals with the optical-to-electric and electric-to-optical *transducers* [1, 10].

Note 1: Optoelectronics should not be confused with electro-optics that deals with alteration of optical properties in response to an applied electric field (see *electrooptic effect*).
Note 2: Optoelectronic effects are *electroluminescence*, *photoconductivity* and *photovoltaic effect*.

2.123 Peierls distortion

Distortion of the perfectly periodic one-dimensional crystal *lattice* due to oscillations of atom nuclei [26].

Note 1: Oscillations of the atom nuclei unavoidably break the perfect order of the ideal 1-D crystal *lattice* without energy barriers with evenly distributed mobile electrons and thus give rise to a *lattice* with energy barriers (*band gaps*) that electrons must overcome to move along the *lattice*. Conversion of the ideal into a real 1-D crystal lattice is called Peierls transition.
Note 2: This quantum-physics theorem was introduced by Rudolf Peierls in about 1930. See also ref. [9].
Note 3: A prototypical Peierls distortion is the bond alternation in *polyvinylene* chains. Valence vibrations of atom nuclei namely make an ideal *lattice* with evenly distributed (perfectly *delocalized*) mobile *electrons* less stable compared to the *lattice* with alternating single and double bonds.



Note 4: *Peierls distortions* together with the insufficient inter-chain transfer of charge carriers are the main reasons for the low electric *conductivity* of undoped linear *conjugated polymers*.

2.124 percolation

Formation of the long-range (infinite) functional connectivity in a disperse system composed of small active particles evenly dispersed in an inactive matrix, which makes the system penetrable for a fluid or current.

Note 1: The term percolation is derived from latin word percōlāre that means to filter. Porous materials in which percolation of pores exists can act as filters (pores are "active particles"). In hydrology and geology percolation relates to a slow penetration of water (liquids) through a porous material.
Note 2: Percolation is achieved at so-called *percolation threshold* and exists above it.

2.125 **percolation threshold** (in a composite material)

Minimal volume fraction of functionally active small particles evenly dispersed in a non-active matrix, at which the long-range (infinite) functional connectivity in the system is achieved.

Note 1: A desired transport through the composite material is not possible below the percolation threshold. Percolation threshold is about 0.3 to 0.35 (by volume) for composites with nearly spherical disperse particles while it can be even below 0.10 for composites with short fibers, depending on the fibers' aspect ratio (the length to diameter ratio).

Note 2: *Electrically conducting polymer composites* composed of carbon black microparticles dispersed in a rubbery matrix are transposed in the electrically conducting state above percolation threshold.

2.126 phonon

Quasiparticle defined as collective excitation associated with a packet of vibrations that can travel in a crystal *lattice* with a definite energy and momentum and thus carry heat and sound through the *lattice* [9]; modified.

Note: See also *polaron* and *soliton*.

2.127 phosphorescence

Luminescence involving the change in spin multiplicity, typically from triplet to singlet or vice versa [9].

2.128 photochromic polymer

Polymer exhibiting *photochromism*.

2.129 photochromism

photochromic effect

Photoinduced transformation of a material, which is photochemically and/or thermally reversible and produces a spectral change, typically but not necessarily in the visible region [7]; modified.

Note 1: A photochromic material has at least two different forms with distinct electronic (UV/vis) absorption spectra, which are thermally stable under ambient conditions for an observable time. Switching between these forms usually occurs due to a photochemical reaction such as cis-trans isomerization, reversible dissociation, or a transfer of an electron (redox reaction), proton, hydrogen or a functional group.

Note 2: A molecule of a photochromic material thermally back-isomerizes to its thermodynamically more stable form at some rate so that a steady-state population of both color forms is established at continuous irradiation. Such state is called the photostationary state. The back isomerization can be sometimes speeded up photochemically; then the overall process is called photochromism of type P while photochromism with purely thermal back-isomerization is dubbed photochromism of type T.

Note 3: See also *electrochromism* and ref. [9].

2.130 photoconducting polymer

Polymer exhibiting *electrical conductivity* or a clear increase in *electrical conductivity* under irradiation.

2.131 photoconductivity

Electric conductivity resulting from *photogeneration* of *charge carriers* [7, 20].

2.132 photodetrapping

Removal of *charge carriers* from traps in the *bandgap* by irradiation.

2.133 photoinduced discharge

Discharging of an electrically charged material by irradiation.

2.134 photoinjection

Charge carrier injection by a process induced by irradiation.

2.135 photoluminescence

Luminescence occurring upon irradiation of a material.

2.136 photoluminescent polymer

Polymer that exhibits *luminescence* upon irradiation [23]; shortened.

2.137 photorefractive polymer

Optically nonlinear polymer that changes refractive index when exposed to light.

2.138 photosensitization

Photochemical or photophysical process mediated by the molecular entity of a photosensitizer that absorbs radiation and transfers excitation energy to the entity of the substance to be altered [7]; modified.

2.139 photovoltaic effect

Phenomenon consisting in converting light to electricity.

2.140 piezoelectric polymer

Polymer that generates an electric field during deformation and, conversely, deforms when exposed to an electric field [23]; modified.

Note: See also *actuator*, *ferroelectric polymer* and *transducer*.

2.141 polarizability, α

electric polarizability

Tensor quantity relating the induced electric dipole moment, p_i, to the applied electric field strength, E [12].

$$\alpha = p_i/E \quad \left(\text{unit: } \mathrm{Cm^2V^{-1}} = \mathrm{A^2s^4kg^{-1}}\right)$$

2.142 polarization density, P

dielectric polarization

Change in electric dipole moment per unit volume of *dielectric material* in response to its exposure to an electric field.

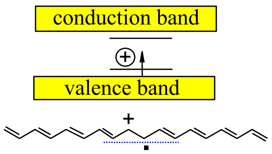
Note 1: The electric field causes limited reversible displacements of charged particles that cannot move freely in the *dielectric material*. **Electronic polarization** (displacements of electrons) takes a femtosecond. So it is in phase with an alternating electric field, such as that of light. **Ionic polarization** (of ions in ionic crystals) is also instantaneous. However **orientation polarization** based on reorientation of permanent dipoles is significantly slower (delayed) and thus often out of phase with the light field.

Note 2: Polarization density (unit $\mathrm{Cm^{-2}}$) is defined as $P = \varepsilon E - \varepsilon_0 E$, where εE (=D) is so-called electric displacement, E the electric field strength, ε_0 the vacuum permittivity and $\varepsilon = \varepsilon_r\varepsilon_0$ permittivity of the *dielectric material*. The ideal dependence of P on E is linear: $P = \varepsilon_0\chi E$, where $\chi = \varepsilon_r - 1$ is electric susceptibility [1, 11]. Non-linearity of this dependence gives rise to *non-linear optical effects*.

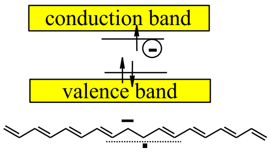
2.143 polaron

Quasiparticle consisting of a *charge carrier* that occupies an energy level in the *bandgap* close to one of its edges and the local *lattice* distortion induced by the accompanying electric field [1, 8, 10].

Note 1: For a chemist, polarons are *radical ions* localized at distorted regions of molecular entities. A positive polaron, P^+, is regarded as a *radical cation* while a negative polaron, P^-, as a *radical anion.*



positive polaron, P^+
charge = + **e**
spin = 1/2



negative polaron, P^-
charge = − **e**
spin = 1/2

Note 2: The electric field of a traveling *charge carrier* polarizes nearby *lattice* elements so causing local lattice deformation accompanying the charge. The work required for this deformation represents an energy barrier that slows down the charge carrier. Periodic *lattice* deformation is defined as *phonon* interacting with the charge carrier and decreasing its *mobility*.

Note 3: A positive polaron (P^+) can be derived by one-electron oxidation while a negative polaron (P^-) by one-electron reduction of a π-*conjugated system*.

Note 4: This definition replaces that one given in ref. [9].

2.144 poling

Orientation of dipoles or dipolar domains inside a material by using a sufficiently strong electric field.

Note: Poling is usually achieved by applying a high strength electric field to the opposite surfaces of a polymer film to obtain *piezoelectric polymer* or *ferroelectric polymer*.

2.145 Poole-Frenkel effect

Increase in the *electric conductivity* of a *semiconductor* or insulator by exposing it to an electric field.

Note: Valence electrons in an insulator or poor semiconductor that is exposed to an external electric field obtain a part of the excitation energy from an external electric field.

2.146 protonic conductivity

hydronic conductivity

Ionic conductivity mediated by protons (more exactly by hydrogen cations properly called hydrons [12]).

2.147 proton doping

hydron doping

Transformation of a semiconducting or insulating material to conducting state by protonation (hydronation) of its molecules.

Note 1: The proton doping is crucial for *polyanilines* that are good conductors only in the protonated state. Deprotonation (dehydronation), as a reverse transformation is achieved by treating the doped polymer with an alkali.

2.148 quantum confinement effect

quantum size effect

Effect occurring if at least one dimension of a structure is comparable to the de Broglie wavelength of the electron-hole pair and the motion of *charge carriers* is thus quantized by the structure boundary [27].

Note 1: A material composed of quantum-size structures exhibits electronic and optic properties different from those of bigger structures. A quantum size effect can be thus detected as an alteration of electronic and optical properties of a solid when reducing its particle size down to nanometer scale.

Note 3: Based on the confinement dimensionality the following quantum-size objects are distinguished:

a) quantum dot: three-dimensional confinement; example: nanoparticles of CdS;
b) quantum wire: two-dimensional confinement; example: carbon nanotubes;
c) quantum well: one-dimensional (linear) confinement; example: nanoscale layer of GaAs sandwiched between two layers of a wide-band-gap *semiconductor* such as AlAs.

2.149 quantum tunneling polymer composite

Electrically conducting polymer composite that, however, is conducting only when pressed due to thinning the insulating polymer matrix membranes so much that they allow *electron tunneling* through them.

Note: Quantum tunneling polymer composites are utilized as pressure *sensors* and touchable control panels of electronic devices. See also *percolation* and *percolation threshold*.

2.150 quantum yield, Φ

quantum efficiency

Number of defined events occurring per photon absorbed by the system [9].

Note 1: Quantum yield as defined above ($\Phi = N_\mathrm{e}/N_\mathrm{fa}$, where N_e and N_fa is the number of events and photons absorbed, respectively) is usually referred to as *integral* quantum yield, Φ_int. Its counterpart is the differential quantum yield defined as the rate of events production divided by the rate of photons absorption: $\Phi_\mathrm{dif} = (\mathrm{d}N_\mathrm{e}/\mathrm{d}t)/(\mathrm{d}N_\mathrm{fa}/\mathrm{d}t)$. These quantities can differ because the events production rate need not be directly proportional to the photons absorption rate. Typical example is photovoltaic conversion, the efficiency of which depends on the incident light intensity.

Note 2: For photo-devices and complex photo-processes, the terms *external quantum yield* (efficiency) and *internal quantum yield* (efficiency) have been introduced [7, 19, 28].

2.151 quasiparticle

Discrete disorder in a multi-particulate system that exhibits particle-specific behavior and properties.

Note 1: A real particle can exist by itself, out of other real particles, while a quasiparticle cannot. It exists only within a multi-particulate system, like a gas bubble inside water or beer. It looks and behaves like a particle, but it does not exist outside liquid. Such a bubble is a macroscopic quasiparticle.

Note 2: Characteristics typical of particles, such as the mass (referred to as effective mass), momentum, energy, velocity, *mobility* and ability to undergo collisions can be assigned to *quasiparticles*.

Note 3: Examples of quasiparticles related to *electromagnetic field responsive* materials are *electron hole, exciton,* magnon, *phonon,* plasmon, *polaron* and *soliton.*

Note 4: There are two main classes of quasiparticles:

a) those of the **excitation type** whose motion corresponds to a motion of individual particles interacting with other parts of the system; examples are *exciton, hole, soliton* and *polaron*;
b) those that originate from a **synchronized collective motion** of the whole system, referred to as collective excitations or collective modes; examples are magnon, plasmon and *phonon.*

2.152 radiative charge carrier recombination

radiative recombination

C*harge carrier recombination* in which the energy released is emitted as a photon of corresponding energy.

Note 1: Radiative charge carrier recombination occurs if a mobile electron meets a *hole* with which it forms an *exciton* that then decays by the radiative electron transition to the ground state.

Note 2: See also *electroluminescence* and *stimulated radiative charge carrier recombination.*

2.153 radical

free radical

Molecular entity possessing an unpaired electron [19, 28]; shortened.

Note 1: The presence of unpaired electrons is indicated by the dot as a superscript at the atom of highest spin density, if this is possible, for example: $H^{\bullet}$ for monohydrogen; $HO^{\bullet}$ for hydroxyl; $^{\bullet}CH_3$ for methyl.
Note 2: The use of the term radical for a substituent group is strongly discouraged [28].

2.154 radical ion

Radical that carries an electric charge [7].

Note 1: A positively charged radical is a radical cation (*e.g.*, benzene radical cation $C_6H_6^{\bullet +}$) while a negatively charged radical is a radical anion (*e.g.*, of benzophenone radical anion $Ph_2C{-}O^{\bullet -}$). The use of terms of the type ion radical is discouraged [28]. The radical must be named first.
Note 2: A radical ion moving or trapped in a *lattice* is, in terms of the solid state physics, referred to as a *polaron*, positive or negative depending on the charge.

2.155 redox doping (of a polymer)

Doping of a parent polymer consisting in oxidation or reduction of its molecules.

Note 1: Redox doping can be accomplished by a chemical reaction or an electrode redox process.

2.156 redox polymer

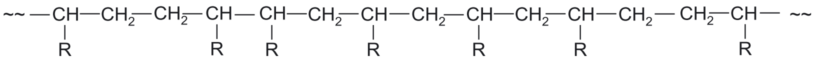
Polymer the molecules of which can be reversibly reduced or oxidized [23].

Note 1: The main-chains and/or the pendant groups of a redox polymer can be oxidized or reduced.
Note 2: *Polyanilines, polyacetylenes* and *polythiophenes* are examples of redox polymers.

2.157 regioirregular polymer

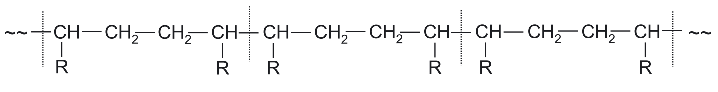
Regular polymer or an *irregular polymer* whose macromolecules contain non-uniformly oriented simple asymmetric repeating units.

Note 1: The difference between regioirregular, irregular and regular chains is shown in the following chart.



$$\sim\sim-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\sim\sim$$

Scheme of a chain of regioirregular vinyl polymer $\left[\mathrm{CHR}-\mathrm{CH_2}\right]_n$ that is also an *irregular polymer.*



$$\sim\sim\Big|\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}\Big|\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}\Big|\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}\Big|\sim\sim$$

Chain of a regioirregular vinyl polymer that can be classified as a *regular polymer* derived from the dimeric repeating unit that is symmetric $\left[\mathrm{CHR}-\mathrm{CH_2}-\mathrm{CH_2}-\mathrm{CHR}\right]_n$(regular HH-TT chain)

Note 2: See also *regioregular polymer* and *head-tail isomerism*.

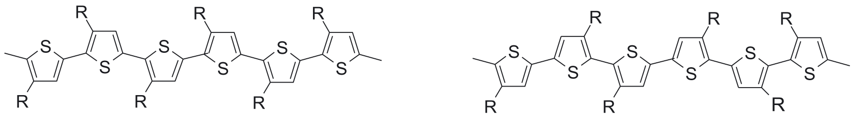
2.158 regiorandom polymer

Regioirregular polymer with randomly oriented asymmetric constitutional repeating units in its chains.

2.159 regioregular polymer

Regular polymer whose chains are composed of uniformly oriented asymmetric constitutional repeating units.

Note: The difference between regioregular and *regioirregular* poly(3-alkylthiophene) chains is as follows:



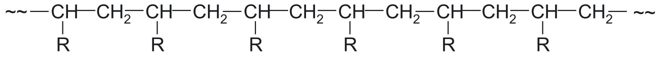
regioregular poly(3-alkylthiophene) chain

regioirregular poly(3-alkylthiophene) chain

2.160 regular polymer

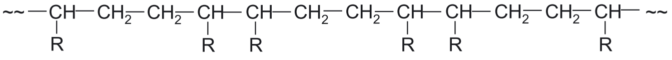
Polymer composed of macromolecules the structure of which essentially comprises the repetition of a single constitutional repeating unit with all units connected identically with respect to the directional sense [25].

Note 1: The difference between regularity and regioregularity of macromolecules is shown in the following chart: See also *head-tail isomerism, stereoregular polymer* and "regioselectivity" in ref. [12].



$$\sim\sim-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\sim\sim$$

regular and also *regioregular chain* of formula: $\left[\mathrm{CHR}-\mathrm{CH_2}\right]_n$



$$\sim\sim-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\underset{\mathrm{R}}{\mathrm{CH}}-\mathrm{CH_2}-\mathrm{CH_2}-\underset{\mathrm{R}}{\mathrm{CH}}-\sim\sim$$

regular, however, regioirregular *chain* of formula: $\left[\mathrm{CHR}-\mathrm{CH_2}-\mathrm{CH_2}-\mathrm{CHR}\right]_n$

2.161 reticulate doped polymer

Surface-*conducting polymer composite* obtained by crystallization of a low-molar-mass organic *conductor* on an insulating or semiconducting polymer support.

2.162 Schottky barrier

Potential energy barrier at a semiconductor-metal junction with the current rectifying characteristics.

Note: The diode based on the Schottky barrier is a Schottky diode or a hot carrier diode. Schottky diodes show switching times down to below 1 ns and a low applied potential drop (0.15 to 0.45 V).

2.163 second harmonic generation

frequency doubling

Transformation of the input monochromatic radiation beam into a double frequency (half wavelength) beam.

Note: Frequency doubling is a *nonlinear optic effect* typical of non-centrosymmetric crystals with a high second-order electric susceptibility. It is utilized in the laser and radio-communication techniques to obtain higher frequency signals, *e.g.*, that of the wavelength 533 nm from the signal of 1066 nm.

2.164 semiconductor

Electric conductor whose *electric conductivity* at ambient conditions is in the range between that of metallic conductors and insulators [13]; modified.

Note 1: A semiconductor can be also defined as a material with non-zero *bandgap energy* up to ca 3 eV.
Note 2: *Electric conductivity* of a semiconductor as well as the *charge carrier concentration* in it can be changed by external factors such as electric field and temperature.
Note 3: The profiles of energy band boundaries are not flat but more or less periodically curved. A simple electron transition within a semiconductor *lattice* is possible only if the valence band top and the conduction band bottom are aligned; this is the case of *direct bandgap semiconductors*. If they are not aligned, the electron transition requires an exchange of a *phonon* of appropriate energy between the electron and the *lattice*, which is the case of *indirect bandgap semiconductors*.

2.165 sensor

Transducer-type device that responds to a specific property of its surroundings or to a coming stimulus by a visually readable change in its state or by generation of a signal that can be read by an observer or instrument.

Note: Examples of sensors are a photodiode, light-emitting diode, pH sensor, air-flow sensor, *etc.*

2.166 short circuit photocurrent, I_{sc}

Photocurrent flowing through a short circuited *solar cell* (if the electric potential across the cell is zero).

2.167 single-strand macromolecule

single-strand polymer molecule

Macromolecule comprising constitutional repeating units connected in such a way that adjacent constitutional units are joined to each other through two atoms, one on each constitutional unit [14, 25, 29].

Note: Single-strand polymers are a subclass of linear polymers.

2.168 singlet state

State having the total electron spin quantum number S equal to zero [7].

Note 1: A singlet state molecule has all electrons paired, so its $S = 0$ and the spin multiplicity (number of spin angular momentum) calculated as $2S + 1 = 1$, which is expressed by the adjective “singlet”.
Note 2: See also *electrofluorescence, electroluminescence* and *triplet state.*

2.169 size effect

Effect of size on properties of the material or device which incorporates it.

Note: See *quantum size effect*.

2.170 solar cell

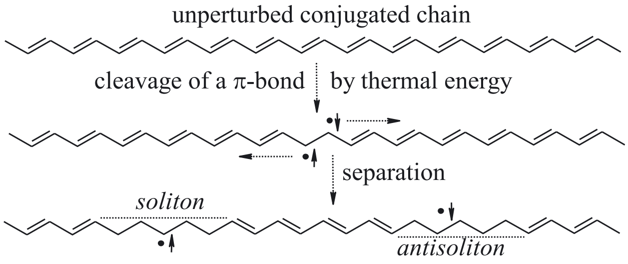
Device that directly transduces electromagnetic radiation into electricity based on the *photovoltaic effect*.

2.171 soliton (general definition)

Self-reinforcing solitary localized wave or wave packet or pulse that maintains its shape while traveling at constant velocity, does not dissipate, and collides with another soliton of the same kind in such a way that it emerges from the collision unchanged, except for a phase shift [30, 31].

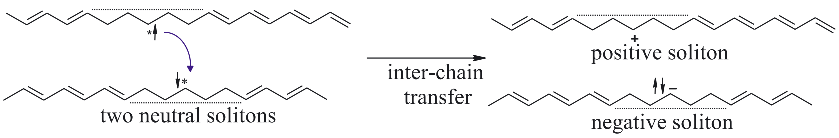
Note 1: In solid state physics solitons are regarded as *quasiparticles* [1, 4–6, 10, 31].

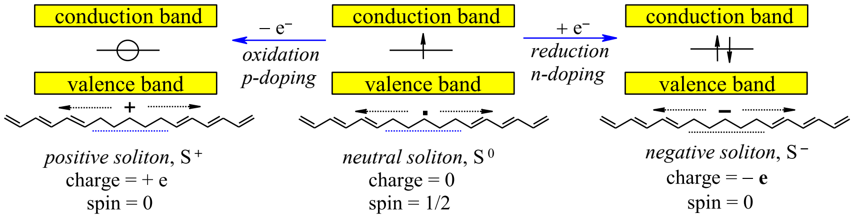
Note 2: Neutral solitons are spontaneously formed as the soliton-*antisoliton* pairs by thermal cleavage of π–bonds in undoped *conjugated polymers*:



If a neutral soliton meets a neutral *antisoliton*, they can radiatively annihilate and form a π-bond.

Note 3: Positive and negative solitons, major *charge carriers* in slightly doped *conjugated polymers*, are formed from neutral solitons by inter-chain *electron transfers* or by their redox doping.





Note 4: A neutral soliton makes an energy barrier between two unperturbed conjugated sequences, whose height is about one half of the *bandgap energy* (compare energy levels of *solitons* and *polarons*). Charged solitons are each associated with the local *lattice* distortion induced by the accompanying electric field (see entry *polaron*).

Note 5: From the chemical point of view, the neutral, positive and negative solitons can be considered as delocalized mobile radicals, cations and anions, respectively.

2.172 stereoregular polymer

Regular polymer composed of macromolecules with configurations defined at all sites of stereoisomerism in the backbone [25]; modified.

2.173 stimulated radiative charge carrier recombination

Radiative charge carrier recombination induced by incident photons of appropriate wavelength, which synchronize emission of other photons as to their wavelength, phase, *polarization* and direction of travel.

Note: If this process takes place in a system with a high population of excited states, it leads to stimulated emission, the principle of the function of lasers.

2.174 thermal injection

Charge carrier injection by a thermally activated processes.

2.175 transducer

Device that converts one type of energy or physical entity to another.

Note 1: A transducer can act as a *sensor*, an *actuator*, or both. Some transducers can operate reversibly in both directions. For example an antenna converts the alternating current into electromagnetic waves and vice versa and an ultrasonic transducer converts alternating current into ultrasonic waves and vice versa.

Note 2: This new definition replaces the one given in ref. [22].

2.176 triplet state

State having the total electron spin quantum number S equal to one [7].

Note 1: A triplet-state molecular species has two unpaired electrons so that its $S = 2 \times \frac{1}{2} = 1$ and its spin multiplicity $2S + 1$ is thus 3. This is expressed by the adjective “triplet”.

Note 3: See also *electroluminescence* and *singlet state*.

2.177 valence band

Highest energy continuum of energy levels in a semiconductor or insulator that is fully occupied by electrons at 0 K [7]; modified.

2.178 valence bond theory

VB theory

Quantum mechanics theory of chemical bonding that treats electrons as being assigned to individual bonds between particular atoms.

Note 1: The VB theory views a chemical bond as a result of weak coupling (overlapping) of atomic or hybridized atomic orbitals or of both and describes *delocalization of electrons* (inherent in *molecular orbital theory*) as a result of resonance mixing of two or more possible energetically equivalent or nearly equivalent structures.

Note 2: VB theory and molecular orbital theory are closely related methods that become equivalent when extended enough. Increasing mixing of VB orbitals gives in the limit extended molecular orbitals.

2.179 work function, Φ

Minimum thermodynamic work (energy) needed to remove an electron from a solid to a point in the vacuum nearby the solid surface.

$$\Phi = -e\Psi - \mu$$

where e is the elementary charge ($-e$ is charge of electron), Ψ is the electric potential nearby the surface and μ is the energy of *Fermi level* [17].

Note 1: Nearby the solid surface means that the released electron remains so close to the solid that it interacts with the surface. Hence the work function depends on the crystal face and contamination.

Note 2: See also *electron affinity*.

3 Survey of typical electronic, photonic and magnetic polymers

This section provides a survey of typical polymers and polymer classes that are currently studied and used as materials for applications in electronics, photonics, sensing and related fields. Structures as well as IUPAC names of the polymers are presented. In this context, it is worth mentioning that there are two types of systematic names of individual polymers used in polymer science: *(i)* **structure-based names** of the generic format poly(CRU), where CRU stands for the name of the constitutional repeating unit [29] the repetition of which in the same directional sense describes a macromolecule of a *regular polymer*, and *(ii)* **source-based names** [32] of the generic format poly(MONO), where MONO stands for monomer(s) from which a particular polymer has been or potentially could be prepared, which are preferably used for polymers whose precise structure is unknown. Besides, there are so-called **polymer class names** [14] that are used for naming polymers of the same structure feature(s) (structure-based polymer class names) or polymers derived from the chemical class of monomer(s) (source-based polymer class names). Polymer class names are generally written without parentheses, for example *polyacetylenes*, *polyanilines*, *polythiophenes etc.* [14], while the name of a particular polymer is generally written with parenthesized part after prefix poly (see the Brief Guide to Polymer Nomenclature [33]). The IUPAC Recommendations related to the polymer terminology and nomenclature published up to year 2008 can be found in ref. [34]. For abbreviations of polymer names and guidelines for their derivation, see reference [35].

3.1 ampholytic polymer

polyampholyte

Polyelectrolyte composed of macromolecules containing both cationic and anionic groups, or corresponding ionizable groups (structure-based polymer class name) [14, 21].

Note: An ampholytic polymer in which ionic groups of opposite sign occur in the same pendant groups is a *zwitterionic polymer*, or *polymeric inner salt*, or *polybetaine*, depending on the structure of the pendant groups.

3.2 fluoropolymers

Polymers whose macromolecules are rich in fluorocarbon groups (structure-based polymer class name).

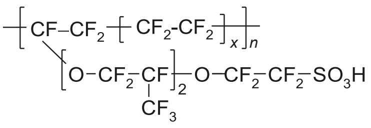
Note 1: This definition replaces that published in ref. [14].
Note 2: Examples of fluoropolymers are:

$$\left[CF_2 \right]_n$$

poly(difluoromethylene)
poly(tetrafluoroethene)

$$\left[CF_2\text{-}CH_2 \right]_n$$

poly(1,1-difluoroethylene)
formerly: poly(vinylidene fluoride)



poly[perfluoro(5,8-dimethyl-3,6,9-trioxaundec-
-1-ene-11-sulfonic acid)-*co*-tetrafluoroethene]
ionomer Nafion™

Note 3: Fluoropolymers are often used as *electrets*. Membranes from *ionomeric* fluoropolymers are used in electrochemical cells.

3.3 ionene

Polymer composed of macromolecules containing ionic groups in the backbone (structure-based polymer class name) [14, 21].

Note 1: Most commonly, the ionic groups of ionenes are quaternary ammonium groups.
Note 2: See also *ampholytic polymer, ionomer* and *polyelectrolyte.*

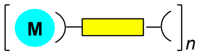
3.4 ionomer

Polymer composed of macromolecules in which a small but significant proportion of the constitutional units has ionic or ionizable groups, or both (structure-based polymer class name) [14, 21].

Note 1: Ionic groups are typically introduced into less than 15 % of monomeric units to cause microphase separation of the bulk ionomer giving ionic domains evenly distributed in the non-ionic, mostly hydrophobic matrix. Ionomers are mostly used as materials for ion-conducting membranes.
Note 2: See also *ampholytic polymer, ionene, polyelectrolyte* and Notes in entry *fluoropolymers.*

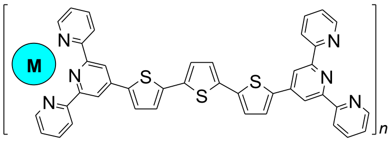
3.5 metallo-supramolecular polymer, MSP

Dynamic polymeric entity whose macromolecules are composed of alternating simple or oligomeric molecules with two or more chelate end-groups (so-called unimers) and metal ions (so-called ion couplers) that are linked to chains by reversible coordination bonds (structure-based polymer class name) [18]:



Note 1: An MSP is spontaneously formed upon mixing unimer(s) with ion couplers, because the activation energy of coordination binding is low. Therefore, the degree of polymerization of MSP is controlled by thermodynamics: it is low in a solution and/or at increased temperature but high in the solid state at room temperature. Due to these features, MSPs belong to the family of constitutional dynamic polymers, so-called dynamers [36]. Constitutional dynamics gives to MSPs processing advantages and capability of self-healing.

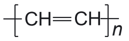
Note 2: Examples are MSPs formed by self-assembly of 2,5″-bis(-2,2′:6′,2″-terpyridin-4′-yl)-5,2′:5′,2″- terthiophene with metal ions M. The MSP with Fe^{2+} ions exhibited *electrochromism* while that with Zn^{2+} ions showed the singlet fission [18].



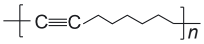
3.6 polyacetylenes

Polymers prepared from acetylene (ethyne), a substituted acetylene, or both in admixture by a polymerization involving one or more triple bonds (source-based polymer class name) [14].

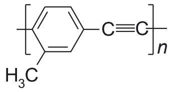
Note 1: Examples of polyacetylenes are:



poly(ethene-1,2-diyl)
formerly: *poly(vinylene)*
poly(acetylene)



poly(oct-1-yne-1,8-diyl)



poly[(2-methyl-1,4-phenylene)-ethyne-1,2-diyl]

Note 2: Polymers of buta-1,3-diyne and its derivatives are a subclass of polyacetylenes referred to as *polydiacetylenes.*

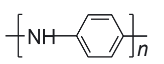
Note 3: Polymers prepared by polycondensations from diols, triols, diamines, dicarboxylic acids *etc.* containing triple bonds (*e.g.,* from but-2-yne-1,4-diol) are excluded. Such polymers are classified as unsaturated polyesters, unsaturated polyamides, *etc.*

Note 4: Although polyacetylenes opened the boom in organic electronics, they did not find commercial application due to insufficient stability under workload and in air. However, polymers of diarylacetylenes are stable and found applications as materials for gas separation membranes [37].

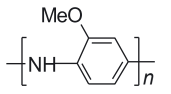
3.7 polyanilines

Polymers prepared exclusively from aniline, or substituted aniline, or both in admixture (source-based class name) [14].

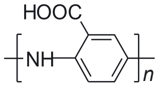
Note 1: Examples of polyanilines (PANI) in the leucoemeraldine base form (see Note 2) are:



poly(azanediyl-1,4-phenylene)
poly(aniline)



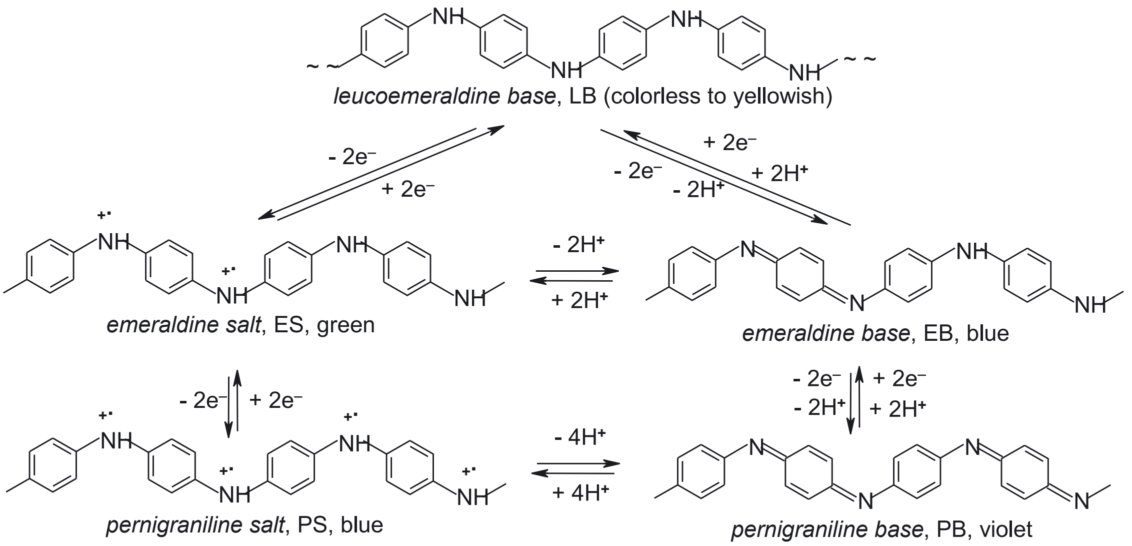
poly[azanediyl(2-methoxy-1,4-phenylene)]
poly(2-methoxyaniline)



poly[azanediyl(2-carboxy-1,4-phenylene)]
poly(2-aminobenzoic acid)

(the first name is the structure-based while the second one is the source-based name of the polymer).

Note 2: Polyanilines exist in various forms (see scheme) differing in the degrees of oxidation (*p-doping*) and protonation (*proton doping*). Gem-based names (leucoemeraldine, emeraldine, pernigraniline) were given to particular PANI forms in 1910 by Green and Woodhead [38].



Note 3: *Redox doping* of PANI-LB by the *electron transfer* (left branch in the scheme) directly gives PANI salts ES and PS, whereas dehydrogenation of LB (right branch in the scheme) gives PANI bases: EB and PB. PANI bases are reversibly transformed to corresponding PANI salts by *proton doping*. The intermediate oxidation state forms, protoemeraldine (product of one-electron oxidation) and nigraniline (product of three-electron oxidation of LB) are sometimes recognized in the literature.

Note 4: PANIs carrying strongly acidic group such as sulfonic or phosphonic group attached to benzene rings are referred to as self-doped PANIs, since the attached acidic groups afford protons ensuring *proton doping* of main chains.

Note 5: The PANI ES form is an *intrinsically conducting polymer* (conductivity of 1–10 Scm^{-1}) in which positive *polarons* and protons are major charge carriers. It is easy accessible by electrochemical or chemical oxidation of anilines in an acidic aqueous medium and it found many applications in electrochemical and photovoltaic cells, batteries, displays and others.

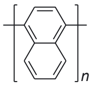
3.8 polyarylenes

Polymers composed of macromolecules containing exclusively arenediyl (formerly arylene) or heteroarenediyl (formerly heteroarylene) units in the backbone:

$$\left[\text{Ar}\right]_n$$

where Ar is a divalent arenediyl or heteroarenediyl group (structure-based polymer class name) [14].

Note 1: An example of a polyarylene is:



poly(naphthalene-1,4-diyl)

Note 2: *Polyphenylenes* (Ar is phenylene or substituted phenylene) are a subclass of polyarylenes.

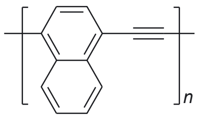
3.9 polyarylenethynylenes

Polymers composed of macromolecules containing exclusively alternating arenediyl or heterarenediyl (formerly arylene or heteroarylene, respectively) and ethynediyl (formerly ethynylene) constitutional repeating units in the backbone:

$$\left[\text{Ar}-\text{C}\equiv\text{C}\right]_n$$

where Ar is a divalent arenediyl or heterarenediyl group (structure-based polymer class name) [14].

Note 1: An example of a polyaryleneethynylene is:



poly[naphthalene-1,4-diylethynediyl]

Note 2: A polymer for which Ar is phenylene is a *polyphenyleneethynylene*.

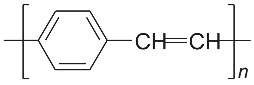
3.10 polyarylenevinylenes

Polymers composed of macromolecules containing exclusively alternating arenediyl or heteroarenediyl (formerly arylene or heteroarylene, respectively) and ethene-1,2-diyl (formerly vinylene) or substituted vinylene constitutional repeating units in the backbone:

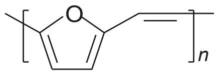
$$\left[\text{Ar}-\text{CR}^1{=}\text{CR}^2\right]_n$$

where Ar is a divalent arenediyl or heteroarenediyl group and R^1 and R^2 are each hydrogen, or an alkyl, aryl or heteroaryl group (structure-based polymer class name) [14].

Note 1: Examples of a polyarylenevinylene are:



poly(1,4-phenyleneethene-1,2-diyl)
poly(1,4-phenylenevinylene)



poly(furan-2,5-diylethene-1,2-diyl)
poly(furan-2,5-diylvinylene)

Note 2: Polyarylenevinylenes are a subclass of *conjugated polymers*. See also *polyphenylenevinylenes*.
Note 3: Polyarylenevinylenes are of interest mainly due to their electroluminescent properties.

3.11 polyazomethines

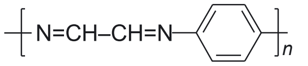
poly (Schiff bases)

Polymers composed of macromolecules containing azomethine (azanylylidenemethanylylidene) linkages in the backbone:

$$-N = CR-$$

where R is hydrogen, or an alkyl or aryl group (structure-based polymer class name) [14].

Note 1: An example of a conjugated polyazomethine is:

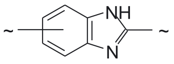


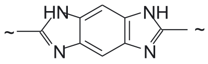
poly(azanylylideneethane-1,2-diylideneazanylilidene-1,4-phenylene)

Note 2: A polymer with only pendant azomethine groups is excluded.
Note 3: The name azomethine is derived from the traditional names "azo" for azanylylidene group –N= and "methine" for the methanylylidene group –CH=.
Note 4: The original distinction between polyazomethines and poly(Schiff base)s, which is that a group R in –N=CR– linkage cannot be hydrogen in a polyazomethine but can be hydrogen in a poly(Schiff base), making polyazomethines a subclass of poly(Schiff base)s, has nearly completely disappeared.

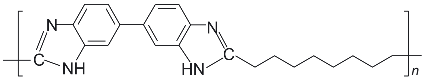
3.12 polybenzimidazoles

Polymers composed of macromolecules containing benzimidazole groups in the backbone, such as groups (structure-based polymer class name) [14].





Note 1: An example of polybenzimidazole is:



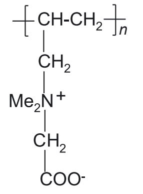
poly([5,5'-bibenzimidazole]-2,2'-diyloctane-1,8-diyl)

Note 2: Polybenzimidazoles are *proton-conducting polymers* with a high thermal stability that found applications as membranes for example in fuel cells or fibers for flame resistant clothes.

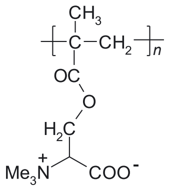
3.13 polybetaines

Polymers prepared from a betaine, i.e., from a zwitterionic monomer containing a trialkylammonium group as the positively charged pole and a carboxylate group as the negatively charged pole (source-based polymer class name) [14].

Note 1: Examples of polybetaines are:



poly(1-{[(carboxylatomethyl)-dimethylammonio]methyl}ethylene)



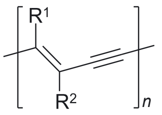
poly[2-carboxylato-2-(trimethylammonio)ethyl methacrylate]
poly[2-(methacryloyloxymethyl)betaine] - source-based name

Note 2: Polybetaines are a subclass of *ampholytic polymer* and of *polyzwitterions*.

3.14 polydiacetylene

Polymer prepared from buta-1,3-diyne (diacetylene) or a substituted buta-1,3-diyne or both in admixture (source-based polymer class name) [14].

Note 1: General formula of a regular polydiacetylene that is prepared by the photo-induced topochemical polymerization of a crystalline 1,3-diyne [38] is as follows:



where R^1 and R^2 are each hydrogen or an alkyl, aryl or heteroaryl group.

Note 2: Polydiacetylenes are a subclass of *conjugated polymers* and of *polyacetylenes*.

3.15 polyelectrolyte

polymeric electrolyte
polymer electrolyte

Polymer composed of macromolecules in which a substantial portion of the constitutional units contains ionic or ionizable groups, or both (source-based polymer class name) [14].

Note 1: The terms polyelectrolyte, polymer electrolyte, should not be confused with the term solid polymer electrolyte which applies to a solution of a low-molar-mass electrolytes in a polymer matrix.

3.16 poly(ethene-1,2-diyl) (structure-based name)

poly(acetylene) (source-based name)
poly(vinylene) (former structure-based name)

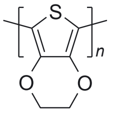
Polymer composed of macromolecules exclusively consisting of ethene-1,2-diyl (formerly called vinylene) constitutional repeating units.

Note: See also *polyacetylenes*.

3.17 poly[3,4-(ethylenedioxy)thiophene] (PEDOT)

poly{3,4-[ethylene-1,2-bis(oxy)]thiophene-2,5-diyl}

Polymer prepared from 3,4-(ethylenedioxy)thiophene (source-based polymer name).



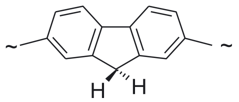
poly{3,4-[ethylene-1,2-bis(oxy)]thiophene-2,5-diyl}
poly[3,4-(ethylenedioxy)thiophene] (PEDOT)

Note 1: PEDOT is an *intrinsically conducting polythiophene* class polymer that is mostly used as a blend with sulfonated polystyrene (PEDOT-PSS), which is produced by oxidative polymerization of 3,4-[ethylene-1,2-bis(oxy)]thiophene (traditional name 3,4-(ethylenedioxy)thiophene, therefore abbreviated as EDOT) in an aqueous solution of partly neutralized sulfonated polystyrene.

Note 2: The PEDOT-PSS is stable in ambient environment, water-dispersible thus processable from aqueous systems and considered as a non-toxic material for the flexible and printed organic electronics and photovoltaics. PEDOT-PSS belongs among the most often used materials for organic as well as organic/inorganic electronic and photovoltaic devices, for antistatic and electrochromic coatings and films, and also exhibits the thermoelectric effect [39].

3.18 polyfluorenes

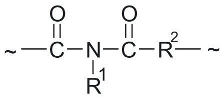
Polymers composed of macromolecules containing fluorenediyl or substituted fluorenediyl (mainly 2,7-diyl) constitutional repeating units in the backbone (structure-based polymer class name) [14].

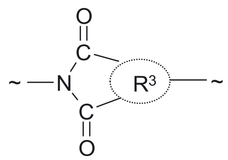


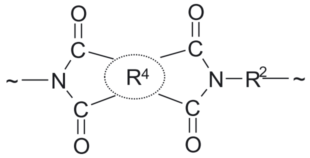
Note: Polyfluorenes are used as photoconducting, photoluminescent and electroluminescent materials for organic light-emitting diodes, organic thin film transistors and polymer solar cells.

3.19 polyimides

Polymers composed of macromolecules containing cyclic dicarboxylmide groupings in the backbone:

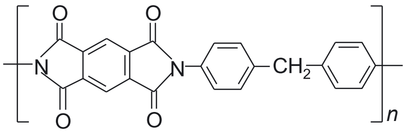






where R^1, R^2, R^3 and R^4 are groups with connectivity one, two, three, and four, respectively (structure-based polymer class name) [14].

Note 1: An example of a polyimide is:

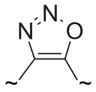


poly[1,3,5,7-tetraoxobenzo[1,2-c;4,5-c']dipyrrol-2,6-diyl-(methylenedibenzene-4,4'-diyl)]
poly[*N,N'*-(methylenedibenzene-4,4'-diyl) benzene-1,2:4,5-bis(dicarboximide)]

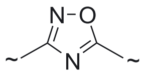
Note 2: In electronics, polyimides are mainly used as highly flexible insulating and passivation layers in integrated circuits and microelectronic chips.

3.20 polyoxadiazoles

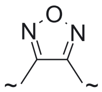
Polymers composed of macromolecules containing exclusively oxadiazole rings in the backbone (structure-based polymer class name) [14].



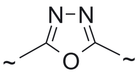
1,2,3-oxadiazole-4,5-diyl



1,2,4-oxadiazole-3,5-diyl



1,2,5-oxadiazole-4,5-diyl

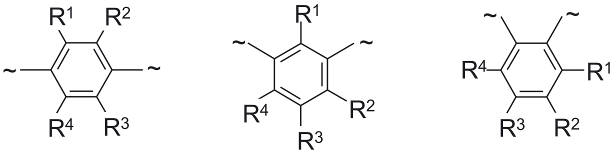


1,3,4-oxadiazole-2,5-diyl

Note: Poly(1,2,3-oxadiazole-4,5-diyl) and poly(1,3,4-oxadiazole-2,5-diyl) are *conjugated polymers*.

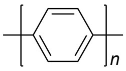
3.21 polyphenylenes

Polymers composed of macromolecules containing exclusively σ-bonded benzene or substituted benzene rings in the backbone:

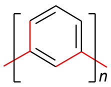


where R^1, R^2, R^3 and R^4 are each hydrogen or an univalent group (structure-based polymer class name) [14].

Note: Polyphenylenes are a subclass of *polyarylenes* and also a subclass of *conjugated polymers* except for poly(1,3-phenylene)s which are not conjugated polymers.



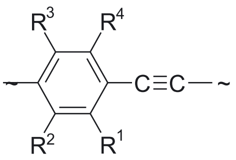
poly(1,4-phenylene)
conjugated

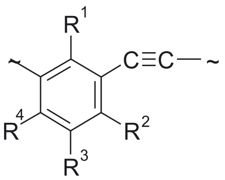


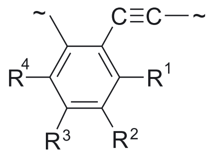
poly(1,3-phenylene)
non-conjugated

3.22 polyphenylenethynylene

Polymer composed of macromolecules containing exclusively alternating phenylene or substituted phenylene and ethynediyl (formerly ethynylene) constitutional repeating units in the backbone:

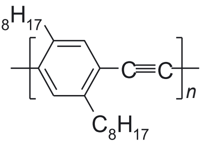






where R^1, R^2, R^3, and R^4 are each hydrogen, alkyl, aryl, halogen, trialkylsilyl *etc.* (structure-based polymer class name) [14].

Note 1: An example of polyphenylenethynylene is:

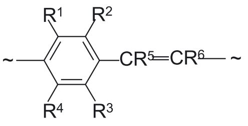


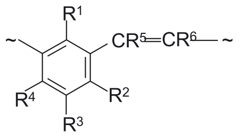
poly[(2,5-dioctyl-1,4-phenylene)ethynediyl]

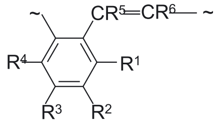
Note 2: Polyphenylenethynylenes are a subclass of *polyarylenethynylenes* and also a subclass of *conjugated polymers* (except for those containing 1,3-phenylene constitutional repeating units).

3.23 Polyphenylenevinylenes (PPV)

Polymers composed of macromolecules containing exclusively alternating phenylene or substituted phenylene and ethene-1,2-diyl (formerly vinylene) or substituted ethene-1,2-diyl constitutional repeating units in the backbone:

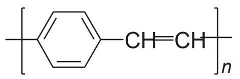






where R^1, R^2, R^3, R^4, R^5 and R^6 are each hydrogen, alkyl, aryl, heteroaryl, halogen, trialkylsilyl, *etc.* (structure-based polymer class name) [14].

Note 1: An example of a polyphenylenevinylene is:



poly(1,4-phenyleneethene-1,2-diyl)
formerly: poly(1,4-phenylenevinylene)

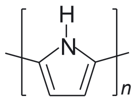
Note 2: Polyphenylenevinylenes are a subclass of *polyarylenevinylenes* and also a subclass of *conjugated polymers* [14].

Note 3: PPVs found applications mainly in the fields of photovoltaic cells and electroluminescent devices.

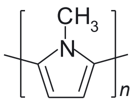
3.24 Polypyrroles (PPy)

Polymers composed of macromolecules with backbones composed of pyrrole rings (structure-based polymer class name definition) [14].

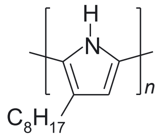
Note 1: Polypyrroles belongs among *conjugated polymers*. Typical examples of PPy are:



poly(pyrrole-2,5-diyl)
poly(pyrrole)



poly(1-methylpyrrole-2,5-diyl)
poly(*N*-methylpyrrole)



poly(3-octylpyrrole-2,5-diyl)
poly(3-octylpyrrole)

Note 2: Polypyrroles found applications mainly in the field of sensors. Applications in electronic devices are still limited owing to insufficient stability of PPy.

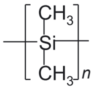
3.25 polysilanes

Polymers composed of macromolecules containing exclusively silicon atoms in the backbone:

$$\left[\mathrm{SiR^1R^2} \right]_n$$

where R^1 and R^2 are each hydrogen or an alkyl, aryl or heteroaryl group (structure-based polymer class name) [14].

Note 1: An example of a polysilane is:



$$\left[\mathrm{Si(CH_3)_2} \right]_n$$

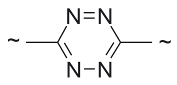
poly(dimethylsilanediyl), formerly poly(dimethylsilylene)

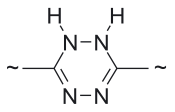
Note 2: Polysilanes were earlier named polysilylenes. A use of this term is discouraged.

Note 3: Polysilanes are σ-*conjugated polymers* which show a good photoconductivity, however, they degrade when exposed to UV light.

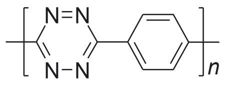
3.26 polytetrazines

Polymers composed of macromolecules containing tetrazine or hydrogenated tetrazine rings in the backbone (structure-based polymer class name) [14]:





Note 1: An example of a conjugated polytetrazine is as follows:

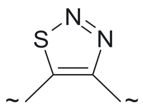


poly(1,2,4,5-tetrazine-3,6-diyl-1,4-phenylene)

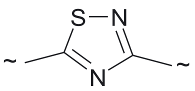
Note 2: A typical polytetrazine contains 1,2,4,5-tetrazine or hydrogenated 1,2,4,5-tetrazine rings since 1,2,3,4- as well as 1,2,3,5-tetrazine rings are unstable.

3.27 polythiadiazoles

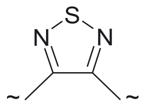
Polymers composed of macromolecules containing thiadiazole rings in the backbone (structure-based polymer class name) [14].



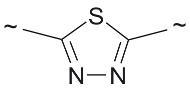
1,2,3-thiadiazole-4,5-diyl



1,2,4-thiadiazole-3,5-diyl

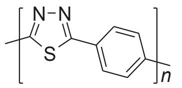


1,2,5-thiadiazole-3,4-diyl



1,3,4-thiadiazole-2,5-diyl

Note 1: An example of a polythiadiazole is:

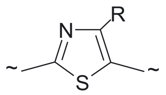


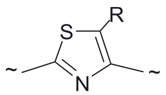
poly(1,3,4-thiadiazole-2,5-diyl-1,4-phenylene)

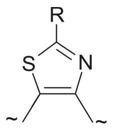
Note 2: Poly(1,2,3-thiadiazole-4,5-diyl) and poly(1,3,4-thiadiazole-2,5-diyl) are *conjugated polymers*.

3.28 polythiazoles

Polymers composed of macromolecules containing thiazole rings in the backbone:

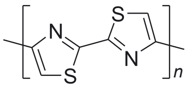






where R is hydrogen, alkyl, aryl, heteroaryl, substituted alkyl, substituted aryl or substituted heteroaryl (structure-based polymer class name) [14].

Note: An example of a polythiazole is:

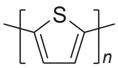


poly{[2,2'-bi(1,3-thiazole)]-4,4'-diyl}

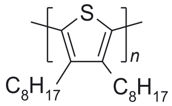
3.29 polythiophenes

Polymers composed of macromolecules containing exclusively thiophene rings in the backbone (structure-based polymer class name) [14].

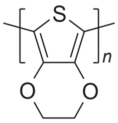
Note 1: Poly(thiophene-2,5-diyl), often written as poly(thiophene), is the generic polythiophene. Examples of polythiophenes and their *structure-based* (first row) and *source-based* (second raw) *names* are:



poly(thiophene-2,5-diyl)
poly(thiophene)

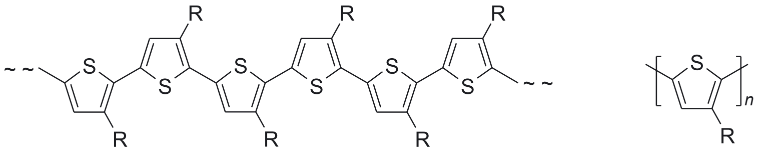


poly(3,4-dioctylthiophene-2,5-diyl)
poly(3,4-dioctylthiophene)

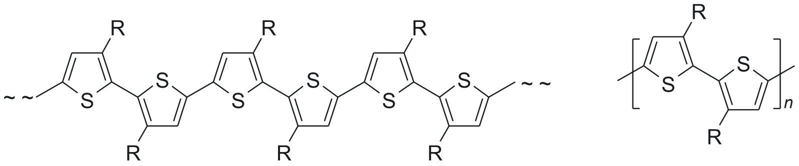


poly{3,4-[ethylene-1,2-bis(oxy)]thiophene-2,5-diyl]}
poly[3,4-(ethylenedioxy)thiophene] (PEDOT)

Note 2: *Regular polymers* of a monosubstituted thiophene are prepared by catalytic coupling polymerization of the corresponding thiophene derivative or its defined dimers (dimers mostly provide *regular* but *regioirregular* polymers, see the chart below). Oxidative polymerization of an asymmetric thiophene monomer gives an irregular polythiophene with considerably worse functional properties.



regular and also *regioregular* poly(3-alkylthiophene-2,5-diyl)

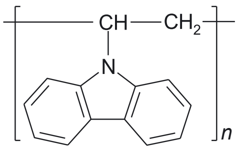


regular but *regioirregular* poly(3-alkylthiophene-2,5-diyl)

Note 4: *Polythiophenes* are a subclass of *conjugated polymers*. The highest practical applications has found poly[3,4-(ethylenedioxy)thiophene] (PEDOT). Regioregular poly(3-alkylthiophenes) are studied as materials for organic *solar cells*. They become conducting upon oxidative *doping*.

3.30 polyvinylcarbazoles

Polymers prepared from a vinylcarbazole or a substituted vinylcarbazole or both in admixture (source-based polymer class name) [14].



poly[1-(carbazol-9-yl)ethylene]
poly(9-vinylcarbazole) poly(*N*-vinylcarbazole)

Note 1: A typical polyvinylcarbazole is poly(*N*-vinylcarbazole) that is usually prepared by a radical or a coordination chain polymerization of *N*-vinylcarbazole.

Note 2: Polyvinylcarbazoles are *photoconducting polymers* that transport charge carriers via carbazolyl pendant groups. They found wide applications, for example, in xerographic photocopying.

3.31 polyvinylenes

Polymers composed of macromolecules containing exclusively ethene-1,2-diyl (formerly vinylene) or substituted ethene-1,2-diyl constitutional repeating units in the backbone:

$$-CR^1 = CR^2-$$

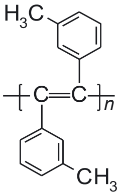
where R^1 and R^2 are each hydrogen or an alkyl, aryl, or heteroaryl group (structure-based polymer class name) [14].

Note 1: Examples of polyvinylenes are:

$-\!\!\left[CH{=}CH \right]_n\!-$

poly(ethene-1,2-diyl)
formerly poly(vinylene)

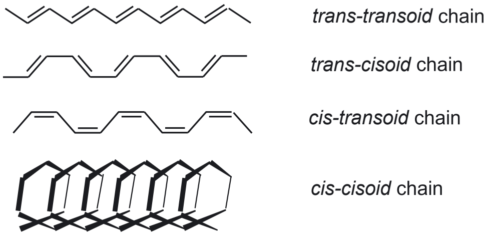
poly(acetylene)



poly[1,2-bis(3-methylphenyl)ethene-1,2-diyl]
poly[1,1'-(ethyne-1,2-diyl)bis(3-methylbenzene)]

(first shown names are the *structure-based* while the second ones the *source-based names*).

Note 2: *Delocalization of electrons* in conjugated chains gives to main-chain single bonds a partial character of double bonds, which restrict free rotations around these bonds which, therefore, show the cis-trans like isomerism. Four basic stereoregular polyvinylene chains can be derived:



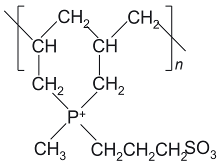
Note 3: Polyvinylenes are almost exclusively prepared by polymerization of acetylene derivatives. Therefore, based on the source, they are mostly *polyacetylenes*.

3.32 polyzwitterions

zwitterionic polymers
polyamphions
poly(inner salts)

Polymers composed of macromolecules consisting of zwitterionic repeating units (structure-based polymer class name) [14].

Note 1: Example of polyzwitterion is:



poly{[1-methyl-1-(3-sulfonatopropyl)-$1\lambda^5$-phosphinan-1-ium-3,5-diyl]methylene}

Note 2: Polyzwitterions are mostly *polyelectrolytes*, since their zwitterionic groups are usually located in pendant groups (not in main-chain groups).

Note 3: *Polybetaines* are a subclass of polyzwitterions.

Note 4: Unlike *polyampholytes*, polyzwitterions have anions and cations in the same monomeric unit.

Note 5: From the chemical structure point of view, a zwitterionic polymer is an *ampholytic polymer* containing ionic groups of opposite sign, commonly in the same pendant group [14, 21].

Membership of sponsoring bodies

Membership of the Subcommittee on Polymer Terminology during preparation of these Recommendations (2006–2019) was as follows:

Chair: R. G. Jones (UK), 2006–2013; R. C. Hiorns (France), from 2014; **Secretary**: M. Hess (Germany) 2006–2007; T. Kitayama (Japan), 2008–2009; R. C. Hiorns (France), 2010–2013; C. K. Luscombe (USA), 2014–2015; P. D. Topham (UK), from 2016; **Members**: R. Adhikari (Nepal); G. Allegra[‡] (Italy); R. Boucher (UK); P. Carbone (Italy); M. C. H. Chan (Malaysia); T. Chang (Korea); J. Chen (USA); C. Fellows (Australia); A. Fradet (France); K. Hatada (Japan); J. He (China/Beijing); K.-H. Hellwich (Germany); P. Hodge (UK); K. Horie[‡] (Japan); A. D. Jenkins[‡] (UK); J.-I. Jin (Korea); J. Kahovec (Czech Republic); T. Kitayama (Japan); J. Merna (Czech Republic); P. Kratochvíl (Czech Republic); P. Kubisa (Poland); S. V. Meille (Italy); I. G. Moad (Australia); W. Mormann (Germany); N. Nakabayashi (Japan); T. Nakano (Japan), C. K. Ober (USA); S. Penczek (Poland); O. E. Philippova (Russia); M. D. Purbrick (UK); G. Raos (Italy); L. P. Rebelo (Portugal); M. Rinaudo (France); G. Russell (USA); C. dos Santos (Brazil); I. Schopov (Bulgaria); C. Scholz (USA); F. Schué[‡] (France); V. P. Shibaev (Russia); S. Słomkowski (Poland); D. W. Smith (USA), R. F. T. Stepto[‡] (UK); N. Stingelin (UK); A. Šturcová (Czech Republic); D. Tabak (Brazil); P. Theato (Germany); J.-P. Vairon (France); M. Vert (France); J. Vohlídal (Czech Republic); M. G. Walter (USA); E. S. Wilks (USA); W. J. Work (USA).

[‡]Deceased

Dedicated to Richard (Dick) G. Jones a long-serving member of the Polymer Division and former Chair of its Subcommittee on Polymer Terminology, and IUPAC Emeritus Fellow. Dick recently passed away on 23 December 2021.

Alphabetical index of terms

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