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IUPAC Recommendations

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Definition of materials chemistry (IUPAC Recommendations 2024)

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Abstract: Materials chemistry is focused on the design, preparation, and understanding of innovative materials. It is an emerging area of research where definitions are not well established. This document defines the area of materials chemistry for the benefit of chemistry communities and the general public worldwide interested in this discipline. This recommendation defines the term "materials chemistry" as the "scientific discipline that designs, synthesizes, and characterizes materials, with particular interest on processing and understanding of useful or potentially useful properties displayed by the materials designed and synthesized for specific applications."

Keywords: advanced polymer materials; biomaterials; definition; design–synthesis–characterization–processing–understanding–utilization; functional materials; materials chemistry; nanomaterials; structural materials.

1 Preamble

This recommendation and its definition of materials chemistry is based on the IUPAC Technical Report of P. Day, L. V. Interrante, and A. R. West.[1] The definition proposed there is continuously and gradually accepted within the chemistry community, confirming the authors' intention that "… in publications where a definition of materials chemistry is required, the proposed definition be used…." However, some inconsistent understandings of materials chemistry persist among parts of the worldwide community, where some scientific journals have not been an exception, which may lead to contextual confusions. This recommendation reflects the findings in the 2009 Technical Report [1] as well as the development since. The current definition term of materials chemistry is recommended to be officially accepted and also included in the *IUPAC Gold Book*.

The most prominent examples demonstrating the growing impact of materials chemistry on interdisciplinary communities are the official scopes of two scientific journals, *Chemistry of Materials* (ACS Publications, ISSN: 0897–4756) and *Journal of Materials Chemistry A, B & C* (RSC Publications, ISSN 2050–7496). The scopes of both journals state that materials chemistry comprises "… focus on the preparation or understanding of materials with unusual or useful properties …"[2] and "… new understanding, applications, properties, and synthesis of materials …."[3] This focus is topical, required, and applied from the point of view of research, development, and application. Such concerted focus has capacity to affect humankind also, as display subjects, contents and feedbacks of the majority of papers appearing in these journals.

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The definition of materials chemistry, and relevant understanding of this growing sector of pure and applied chemistry, is also promoted by the IUPAC, cf. the link to Materials Chemistry Education [4] on the webpage of IUPAC Interdivisional Subcommittee on Materials Chemistry.[5] The rule is that a new definition is endorsed in an IUPAC recommendation. Only a verified and increasingly accepted definition is recommended and further promoted to the broadest audience possible through the worldwide network of IUPAC. Understandings (and definitions) of core areas of chemistry need to be clearly formulated and agreed upon in communities of chemists as well as in general public. This also concerns the emerging area of materials chemistry. Inconsistent understandings or definitions in education and research make the communication difficult. Thus, an agreed-upon and unified definition of “materials chemistry” may prevent confusions and provide common language in this area.

2 Definition, notes, and rationale

The history and current status of the research and teaching, only a few decades ago labeled as materials chemistry, have been analyzed and described in the IUPAC Technical Report.[1] The report gives evidence that “the field has become one of the growth sectors in pure and applied chemistry.” However, it also marks that in the period of publishing the report, there has been (i) “no consensus regarding a definition for the subject” and (ii) “a danger of considerable confusions what does/does not fall within the scope of materials chemistry.” The authors of the report[1] have provided a thorough analysis of the entire topic and proposed the definition of materials chemistry. Subsequently, the definition has been gradually accepted within the chemistry community.

Attitudes and achievements in the fields of materials science and materials chemistry in course of one and half decade following the 2009 Technical Report have been analyzed for purposes of this recommendation. A definition for the term “material” can be found elsewhere, a broadly accepted one in ref. 6. A growing importance of research and educational topics labeled as materials chemistry has been noted across online resources, new or re-edited textbooks, and especially from the annual growth of the number of papers published in the related scientific journals. The current status of the research and teaching enables defining materials chemistry as the scientific discipline focused toward both the design and synthesis of materials and the understanding of acquired properties that are a challenge for developing materials with novel applications. The definition term is recommended to be officially accepted and also included in the IUPAC Gold Book. Wording of the definition closely relates to that proposed in the IUPAC Technical Report[1] but also generalizes the development since. Notes that supplement the definition have been added (reflecting as the quoted report so the newest development in the field).

2.1 Materials chemistry

Materials chemistry is the scientific discipline that designs, synthesizes, and characterizes materials with particular interest on both their processing and the understanding of useful or potentially useful properties displayed by the materials designed and synthesized for specific applications.

Note 1: The aspects of design, synthesis, and function (useful or potentially useful properties) are all needed for the topical item of material research/development/production to be part of materials chemistry.

Note 2: The keywords “useful” and “properties” emphasize functionality as a major driving force of the practitioners of materials chemistry.

Note 3: For a series of further details on both the structure-property relation and functionality by design, read below in this recommendation and in the source.[1]

A selection of examples and the rationale underpinning the cross-disciplinary nature of materials chemistry are given below. Much of materials chemistry is motivated by discovering and developing materials for desired applications. Whilst this is an essential motivating factor, the need to develop the structure–property relation is crucial for any category of chemicals to be a material useful for the well-being of humankind. Key tools of practitioners of materials chemistry are chemistry-based approaches in general. Work that considers only the synthesis and characterization of new chemical substances is simply chemical synthesis, not materials chemistry. Synthesis and characterization of new chemical substances with additional inherent focus on its properties useful to humankind is considered materials chemistry.

There are several successful examples of educational resources for solid state and materials chemistry, such as online resources in the IUPAC webpage of Materials Chemistry EDU,[4] or textbooks[7–9] that provide a common language for teaching in the area. The introductory chapters of Woodward et al.[7] cover topics such as crystal structures, defects, diffusion in solids, chemical bonding, and electronic band structure. The textbook further navigates the reader toward the examples and to the understanding why and how the useful properties of materials can ultimately be traced back to structure and dynamics at the atomic level and also controlled from this level. Also new editions of textbooks are valuable educational tools[8,9] that can concisely document how the central role of chemistry in materials science stems from the ability to design and synthesize new materials with properties previously never observed. For example, individual chapters of Fahlman's textbook[9] conclude with sections describing important material applications as well as addressing thought-provoking questions to readers.

The report of P. Day et al.[1] states that "… synthesizing a new chemical substance in nano- or macroscopic form is not materials chemistry but just chemical synthesis … to be considered materials chemistry there needs to be an element of application, function, or design …." In general, the features of application, function, and design serve to discern a "material" from a "chemical." The progress of knowledge about nanomaterials and potentially useful properties and application of these is justified also by further detail: nanomaterials and their properties represent specific fields in which, besides the design, synthesis is already implicit in the topic. The main purpose of their synthesis is to control both the surface area of nanomaterials and the size of nanoparticles below 100 nm or even below 10 nm. Such small nanoparticles have very different physicochemical and biophysical properties and therefore also different application/function and potential when compared to the bulk material.

This and the next paragraphs quote several focused examples and topics within the field of materials chemistry. Structural details provide a series of structure–property relationships topical in materials chemistry.[1,7–9] An example with long history, referred also in ref.[1], provides the construction industry with solutions based on recent research in this area. The compound Ca_2SiO_4, especially its polymorphs affecting the formation of concrete from cement, illustrates the role of structural modifications[10] on properties. The γ-polymorph reacts with water negligibly, yet its reaction with CO_2 dissolved in water may increase the strength of concrete.[11] The β-polymorph of Ca_2SiO_4 in Portland cement reacts quickly with water, the added value of materials chemistry in novel cement-based materials is the knowledge on the cross-linking of selected atoms of cement and polymer,[12] while strength of the material[10–12] is a challenge. This example illustrates how the construction industry, and much of its novelty, rest on the detailed packing arrangement of the atoms in components of cement and its partner compound.

Topical up-to-date cutting-edge research and development on the structure–property relationships in the field of materials chemistry include research in polymer materials.[1] By focusing on the structure and elemental composition with an eye toward properties, polymers are viewed as molecular materials where useful collective properties result from the interactions between individual component molecules. Furthermore, organic groups on polymers can be modified to control physical and chemical properties. Polymer materials, including the design and synthesis of derivatives of biopolymers, are utilized in a variety of technological applications.[13] Applications include, but are not limited to, solid-state batteries, composite materials (including micro-structured meta-material designs), isotropic transparent polymeric materials, organic light-emitting diodes, nonlinear optics, and also biomedical applications or water treatment technologies.

The fast-growing field of biomaterials is an area of challenge in materials chemistry. Entirely synthetic or derivatives of natural, with or without an organic component, biomaterials interact with biological systems and are mostly used in tissue engineering and medicine to replace, regenerate, repair, or augment any body part in terms of structure and/or function. Sometimes these may also satisfy an aesthetic demand. While biomaterials do not fulfill the function of a drug, the issue and potential impact of materials chemistry in this field (besides abovementioned functions) is also in the design and development of biomaterials in drug delivery systems. Thus, typical and common biomaterials, and also novel synthetic materials examples, exert useful or potentially useful bio-relevant properties and functions.[14–19] The examples comprise (i) metals and alloys, such as Ti-, Mg-, or Ta-based alloys for bone fixation and joint replacements; (ii) ceramics, such as alumina, zirconia, calcium phosphates, hydroxyapatite for bone cement, and dental implants attached to the tooth; (iii) polymers, such as polyethylene, polymethylmethacrylate, silicones, hydrogels for contact lenses, implants, and artificial ligaments; and (iv) oxides and nonmetallic elements, such as SiO_2, iron oxides, carbon for abrasive components of skin care products, and tattoo colors. Biomaterials should not be confused with biominerals – naturally occurring minerals integrated in the body of organisms.[18] The important group of biomaterials contains also naturally occurring biopolymers,[14,15,19,20] such as cellulose, silk, chitosan, collagen, hyaluronan, elastin, and alginate. However, due to the fact of natural occurrence (and thus no design nor synthesis needed), these should not be considered the topic of materials chemistry.

Another large area of research is perovskites and perovskite-based materials which has grown because of the prominent impact of chemistry-based approaches on materials properties and functionality. The current pace of research and innovation[21] spans from tailoring the composition to controlling functionality, as for example in the photovoltaics sector. Perovskites are generally described with the chemical formula ABX_3 (typically A and B are metal cations and X is an anion). The structure is robust so that perovskite materials can host a large variety of constituents to affect properties and potential of application. Perhaps the most prominent applications of perovskite materials are solar cells and photovoltaics in which the selection of perovskite material can effectively determine the cell efficiency.[21]

A recent example is based in sonochemistry, which is the use of (ultra)sonic waves to trigger chemical reactions. Sonochemistry exerts huge potential to manufacture innovative functional (nano)materials and coatings with magnetic, fluorescent, and antimicrobial properties.[22–25] The sonogalvanic method has been reported to effectively modify the surface of porous silicon by palladium nanoparticles.[26] As an emerging technology, sonochemical coatings may be in future a route toward safer, more durable materials with value-added properties. For these reasons, possibilities are explored to scale up this method to an industrial setting that will enable continuous production of coated materials.[25]

3 Conclusions

The role of chemistry-based approaches is gradually increasing as materials with useful or potentially useful properties and applications for the well-being of humankind become the subject of interest of practitioners of materials science and materials development. A definition of materials chemistry is recommended in wording that is closely related to the 2009 IUPAC Technical Report of P. Day et al.,[1] and generalizes the development since. The definition introduces a common language into the emerging area of materials chemistry for teaching, research, or applications. The definition, together with the notes and a selection of examples, rationalizes the field and underpins the cross-disciplinary nature of materials chemistry. It has the potential to overcome confusion due to inconsistent understanding of materials chemistry and its role in the development and use of new materials.

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