Beyond Classical Chemistry:
Subfields and Metafields of the Molecular Sciences

by Jesper Sjöström

The boundaries between both basic research and engineering and between the classical sciences are becoming increasingly blurred. This is partially a consequence of the increased interaction between science and society. For chemistry, the blurring of boundaries and an increased emphasis on applications have led to the emergence of two "super-sciences," material sciences and biomolecular sciences, respectively. In these, chemistry is only a part, although an important one. The increased interaction between chemistry and society has also resulted in the emergence and development of metadisciplines such as green chemistry, chemistry education, and the philosophy of chemistry. This article discusses—based on "knowledge maps" of chemistry—ongoing trends in the molecular sciences (MS). As a consequence of the more application-oriented research—mainly to do with medicines, new materials, and the environment—the position of chemistry as an independent discipline has become indistinct.

Classical Chemistry	Molecular Sciences
"academic chemistry"	**"post-academic chemistry"**
• Classical subdisciplines: organic chemistry, inorganic chemistry, analytical chemistry, physical chemistry, biochemistry	• Interdisciplinary fields: material sciences and biomolecular sciences (chemistry as a service discipline)
• Chemistry has a disciplinary self-value (in addition to its usefulness)	• Application focus: blurring boundary between science and technology
• Research organizations subdivided according to the classical subdisciplines	• Interdisciplinary research centers and industry-sponsored research programs

Table 1. Comparison between Academic and Post-Academic Chemistry.

From Academic to Post-Academic

The research practice of chemistry has changed tremendously during the last few decades, not only in the laboratory—due to advances in instrumentation—but also in the organization of research. Especially since WWII, chemistry has been influenced by physics on the one hand, and biology and medicine on the other hand. Physics has influenced both theories and experimental methods of chemistry, and is the basis for the revolution in instrumentation. From the 1950s one can talk about a "physicification" of chemistry. Similarly, one can talk about a "biofication" of chemistry from the 1970s. Biology and medicine have had a huge effect on the choice of research questions in chemistry. Furthermore, the development of gene and computer technologies have had big influences on the research practice of chemistry.

The identity, rhetoric, and organization of chemistry have shifted from an "academic" mode to a more application-oriented mode ("post-academic chemistry"), which is driven as much by the surrounding society as by the chemistry community itself (see Table 1). The dichotomy of *academic* and *post-academic* is borrowed from Ziman.[1] Chemistry after WWII has been different in three ways: (1) research has become increasingly more specialized in parallel with the blurring of the boundaries with other disciplines,[2] (2) the revolution in instrumentation has had a big influence on the research practice,[3] and (3) new patterns of collaboration between academia and industry have developed. These trends are both a consequence of and a reason for the "physicification" and "biofication" of chemistry.

1. Ziman, J. (1994) *Prometheus Bound—Science in a Dynamic Steady State.* Cambridge: Cambridge University Press; Ziman, J. (2000) *Real Science—What It Is, and What it Means.* Cambridge: Cambridge University Press.
2. Reinhardt, C. (ed.) (2001) *Chemical Sciences in the 20th Century—Bridging Boundaries.* Wiley-VCH
3. Morris, P.J.T. (ed.) (2002) *From Classical to Modern Chemistry—The Instrumental Revolution.* RSC, Science museum och CHF.

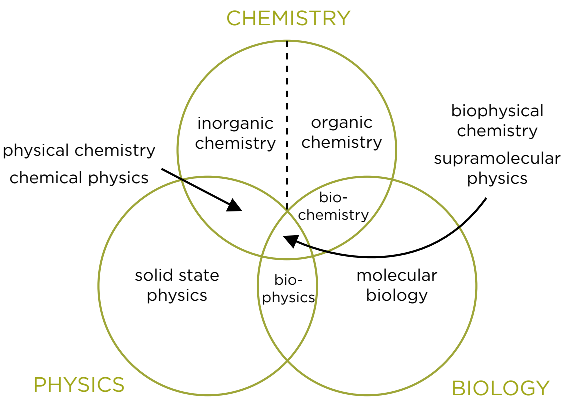


Figure 1: A "knowledge map" for chemistry.

Knowledge Maps of Chemistry

Traditionally "pure" chemistry is seen as situated inbetween physics and biology. In Figure 1 a somewhat more complex "knowledge map" is shown. In the boundaries have evolved subdisciplines such as physical chemistry and biochemistry. These two—together with organic chemistry, inorganic chemistry, and analytical chemistry—are often seen as the five classical subdisciplines of chemistry. As a result of the "physicification" and "biofication" of chemistry, new fundamental subdisciplines such as theoretical chemistry and macromolecular chemistry have complemented the classical five.

Chemistry as a discipline has changed a lot during recent decades. The U.S. National Research Council's (NRC) 2003 report on the future of the field noted that "Chemistry and chemical engineering have changed very significantly [...] They have broadened their scope—into biology, nanotechnology, materials science, computation, and advanced methods of process systems engineering and control—such that much of what is done and taught in chemistry and chemical engineering departments is now quite different from the classical subjects."[4] Today it is application-oriented fields, such as nanotechnology, polymer technology, biotechnology, and biomedicine, that are regarded as hot. All of these fields are problem-oriented and interdisciplinary. Therefore, they are crossing the border between science and technology. Baird and Schummer write: "[T]he nanotechnology movement spreads across the disciplines and ignores classical boundaries [...and] the boundary between science and technologies increasingly blurs."[5]

Figure 2 shows a more modern knowledge map. In the boundary between applied chemistry and physics one finds materials science. Similarly, biotechnology is situated in the intersection between applied chemistry and biology. More generally, it is the two supersciences, material sciences and biomolecular sciences, that we find in the intersections. In the intersection between the two supersciences has evolved the field of bionanotechnology. This is for the moment a hot area, which can be illustrated by the fact that Elsevier launched the journal *Nanotechnology, Biology, and Medicine* in the beginning of 2005. In addition to bionanotechnology, a large part of surface and colloid technology also is situated in the boundary between the two supersciences. Other examples are biosensors and artificial photosynthesis. It is interesting to note that for several years chemical research at Uppsala University in Sweden has been subdivided according to the supersciences; bioresearch and material-oriented research are performed in two distinct interdisciplinary research centers.

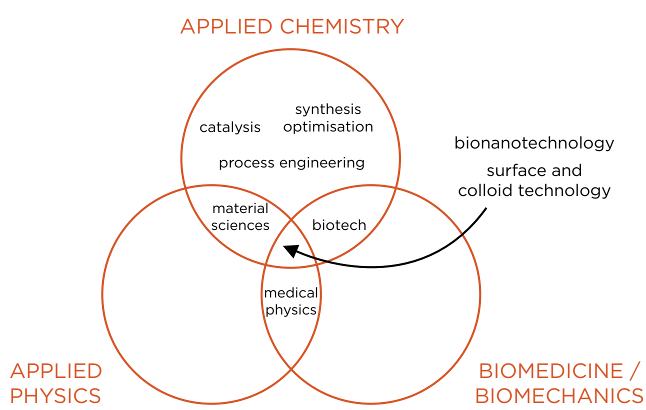


Figure 2: A revised—more modern—"knowledge map" for chemistry.

During the last decade, several authors and policy documents have stated that synthesis (and catalysis), biotechnology (and biomedicine), materials sci-

4. NRC (2003) *Beyond the Molecular Frontier: Challenges for Chemistry and Chemical Engineering.* Committee on Challenges for the Chemical Sciences in the 21st Century, National Research Council. Washington: The National Academies Press, p. 11.

5. Baird, D.; Schummer, J. (2004) *"Editorial: Nanotech Challenges, Part I" HYLE—Int. J. Phil. Chem.* 10(2):63-64.

ences, and environmental technology will be important research areas in chemistry in the future.[6] With this as a basis, Figure 3 shows a model over the molecular sciences. In the middle one finds *the core* of chemical knowledge (i.e., chemical synthesis, chemical theory, and chemical method development). The latter should be understood broadly to encompass instruments, computational chemistry, and process technology. In *the boundaries* one finds the supersciences of material sciences and biomolecular sciences, respectively. The diffuse borders between chemistry and other knowledge fields in these supersciences are symbolized with the purple circle, covering the knowledge area of classical chemistry.

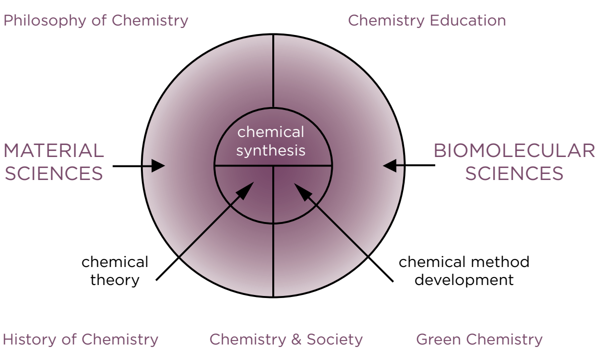


Figure 3: A knowledge map for molecular sciences and metadisciplines.

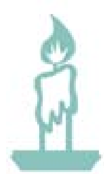
New medicines and the environment are recurring themes in much of modern chemical research. Much synthetic chemistry is today oriented towards medicinal chemistry, with some research aimed at developing "green chemicals." Similarly, within material sciences, research is directed toward new drug delivery systems and "green materials." For the biomolecular sciences, most research is aimed at finding new drugs. However, during recent years, scientists in this field have been exploring using biotechnology for environmental remediation and protection.

6. ACS; ACC; AIC*hE; CCR; SOCMA (1996)* Technology Vision 2020: The U.S. Chemical Industry. Washington, D. C. (Executive Summary: <www.ccrhg.org/vision/>; AIIChemE (1996) *Chemistry—Europe & the future* <www.cefic.be/allcheme>; vide supra, reference 4; SusChem (2005) *A European Technology Platform for SUSTAINABLE CHEMISTRY—The vision for 2025 and beyond*. Final Draft, endorsed at a stakeholder event in Barcelona, 4 March 2005.

Metachemistry

In addition to the real molecular science subdisciplines, the model in Figure 3 also indicates the presence of several metadisciplines, of which some have developed a lot during the last decade. Together, I call these metadisciplines *metachemistry,* which can be understood as the meeting of knowledge between chemistry and different subareas of the humanities. The five chemical meta-areas are the philosophy of chemistry, chemistry education, history of chemistry, chemistry and society, and green chemistry. Below I describe these areas in more detail.

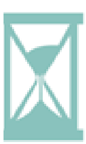
The five metachemical knowledge fields and the chemists within them, which aim at contextualizing and analyzing chemical practice, have so far been relatively separated from each other. However, these fields must become a natural part of chemistry curricula, and become integrated in chemists' and chemistry teachers' reflectivity and practice. Clearly, there is a need for more coverage of metachemical disciplines in chemistry courses as a result of the increased interaction between science and society.



Philosophy of Chemistry is a metadiscipline on the border between chemistry and philosophy of science. It mainly deals with the nature of chemistry and its disciplinary boundaries (epistemological, methodological, and metaphysical reasoning), but also to some extent the culture of chemistry, its aims, and its disciplinary identity. Furthermore, questions about chemical ethics[7] and aesthetics are discussed. Although chemistry is a large science that has had a big influence on all other experimental sciences, the philosophy of chemistry in a modern sense is a very new area; it was formed as a research field in the mid 1990s.[8] In 1997 the International Society for the Philosophy of Chemistry was founded, and at about the same time two journals were launched: *HYLE—International Journal for Philosophy of Chemistry* and *Foundations of Chemistry*. To quote Schummer, "ironically, philosophy of chemistry emerged at a time when scientific activities increasingly transcended disciplinary boundaries towards problem-oriented research."

7. See especially: Special Issues on 'Ethics of Chemistry' in *HYLE—Int. J. Phil. Chem.* (2001/2002) vol. 7(2) and 8(1).
8. Schummer, J. (2003) *"The philosophy of chemistry" Endeavour* 27(1):37-41.

Chemistry Education is a metadiscipline on the border between chemistry and the educational sciences.[9] It has a long history, but has to some extent changed its character during recent decades. Chemistry education deals with question such as why and how to teach chemistry. Furthermore, it deals with the question of appropriate curriculas. Three different types of knowledge can be regarded as important to the teaching chemistry: (1) "ontological" (i.e., real chemistry), (2) "epistemological" (i.e., philosophical and cultural perspectives on the chemical enterprise), and (3) "ethical" (i.e., problematization of the role of chemistry in society).[10] Historically, ontological knowledge has been the main focus of this field. The traditional focus of this field has been on unproblematizing learning, but recently there has been increasing emphasis on more contextualized chemistry teaching,[11] ethical perspectives,[12] philosophical perspectives,[13] and the connection to environmental education.[14] Johnstone's triangle, which contains symbolic, molecular, and macroscopic levels, has been complemented by Mahaffy with a humanistic dimension, emphasizing both real-life problems in the interface between science and society and the importance of putting the student in the center.[15] Important journals in this field include the *Journal of Chemical Education* and *Chemistry Education: Research and Practice.* Furthermore, many articles in the field are published in more general science education journals.



History of Chemistry is a metadiscipline on the border between chemistry and the history of science. It has a long history, but has—similarly to chemistry education—changed its character during recent decades. It is possible to identify four different subtypes within the history of chemistry field: (1) history of the science, (2) history of chemistry teaching, (3) history of the industry, and (4) history of the environment. In September 2005 in Portugal, the section for History of Chemistry within the European Association for Chemical and Molecular Sciences held the 5th International Conference on the History of Chemistry on the theme "Chemistry, Technology, and Society." In other words, modern history of chemistry tries to place the science in technological and social contexts. However, the journals *AMBIX: The Journal of the Society for the History of Alchemy and Chemistry, Chemical Heritage,* and *Bulletin for the History of Chemistry* mainly deal with old chemistry.

Chemistry and Society is the knowledge area on the border between chemistry and society. This field has two areas of focus: (1) "chemistry-as-society" (i.e., the chemical communities), and (2) "chemistry-in-society" (i.e., the use and effects of chemistry in society). It is an area where the values and perspectives of the authors have a big influence on the positions presented. There tend to be three general perspectives in the debate over chemistry and society: (1) persons from academia arguing for more and better basic chemical research, (2) politicians and persons from industry arguing for more focus on chemical innovations, and (3) persons with an analytical perspective[16] influenced by the research area STS (Science and Technology Studies). It is often the latter perspective that is the basis for university courses in chemistry and society.[17] This article can also be regarded as an example of the latter perspective. An example of the second perspective is a section about chemistry and society that appeared in a European report that argued that chemical research and chemists are important for future economic growth.[18] News magazines that cover this field include

9. Tsaparlis, G. (2003) "Globalisation in Chemistry Education Research and Practice" *Chemistry Education: Research and Practice 4*(1):3-10.
10. Krageskov Eriksen, K. (2002) "The Future of Tertiary Chemical Education—A Building Focus" *HYLE—Int. J. Phil. Chem.* 8(1):35-48.
11. Zoller, U. (2000) "Interdisciplinary systemic HOCS development—The key for meaningful STES oriented chemical education" *Chemistry Education: Research and Practice in Europe* 1(2):189-200.
12. Kovac, J. (1996) "Scientific Ethics in Chemical Education" *J. Chem. Education* 73(19):926-928.; Kovac, J. (1999) "Professional Ethics in the Collage and University Science Curriculum" *Science and Education* 8:309-319.; Coppola, B. P. (2000) "Targeting Entry Points for Ethics in Chemistry Teaching and Learning" *J. Chem. Education* 77(11):1506-1511.
13. Erduran, S. (2001) "Philosophy of Chemistry: An Emerging Field with Implications for Chemistry Education" *Science & Education* 10:581-593.
14. Zoller, U. (2004) "Chemistry and Environmental Education" *Chemistry Education: Research and Practice* 5(2):95-97
15 Mahaffy, P. (2004) "Tetrahedral Chemistry Education: Shaping What is to Come" *Chemistry International* November-December, p. 14-15; Mahaffy, P. (2004) "The Future Shape of Chemistry Education" *Chemistry Education: Research and Practice* 5(3):229-245.
16. Vide supra, reference 11.
17. Schwartz, A.T.; Bunce, D.M.; Silberman, R.G.; Stanitski, C.L.; Stratton, W.J.; Zipp, A.P. (1994) *Chemistry in Context: Applying Chemisty to Society.* Brown: Dubuque.; Andersson, S.; Sonesson, A.; Vannerberg, N.G. (1999) Kemin i samhället. Liber: Stockholm (in Swedish).
18. AllChemE (1996) *Chemistry—Europe & the Future* <www.cefic.be/allcheme>.

Chemistry International, Chemistry World, Chemical Week, and *Chemical Market Reporter.*

Green Chemistry is a metadiscipline on the border between chemistry and industrial ecology.[19] It is based on 12 widely spread principles[20] that cover most of chemistry and chemical engineering.[21] The main principle is prevention. The other principles can be summarized in the following way: (1) renewables as chemical feedstocks, (2) substitution of hazardous chemicals, and (3) reduced consumption of chemicals and energy. More generally, green chemistry is about creating a more environmentally friendly chemistry practice, from the laboratories to chemical production to chemicals in society.[22] The green chemistry movement started in the USA in the early 1990s and has since spread all over the world.[23] The number of scientific publications with the key word "green chemistry" has increased substantially during the last five years. The main journal for the metadiscipline is *Green Chemistry,* which was launched in 1999. However, several journals have had special issues about the area during the last five years. It is interesting to note that green chemistry is the metafield that is most closely related to real chemistry. Most of its practictioners are also active as chemists. The relationship to real chemistry is indicated by the fact that green chemistry is the only metadiscipline that was discussed in the NRC report mentioned previously,[24] although the importance of good science education also was emphasized.

Future of Chemistry

After considering the different metafields in modern chemistry, it is interesting to again look at real chemistry research and try to say something about the future of the discipline. Today there are signs that "chemist" as a professional identity is losing its former strength. The reason is that chemistry has become more specialized, has mixed with other sciences, and has become more oriented towards applications. As a result of this transformation of chemistry, Nye's definition of disciplinary identity is no longer applicable to chemistry. She writes, "Scientific disciplines identify new problems and solve them. This happens within well-established disciplines and within areas of investigation that become new specialities or disciplines. It is the shared problem-solving activity [...] that [...] prolongs the disciplinary identity."[25] Modern chemistry is working with a complex mix of different problems. Therefore, today the different subdisciplinary identities are more important than a common "chemist" identity.

"Chemistry" as a term does not encompass as many research fields as it did in the 1960s. As a result of first the physicification and then the biofication of the field, "chemistry" as a discipline is both very broad (including both biochemistry and physical chemistry in a broad sense) and rather limited (mainly the core of chemistry, synthetic chemistry with its molecule makers) at the same time. There are signs that chemistry in the future mainly will be a service discipline to the life sciences and other interdisciplinary fields. To cover the broader area, where classical chemistry is the core, but not the whole knowledge base (remember Figure 3), there are a number of examples where "chemistry" is being exchanged with—or at least complemented with—the broader "molecular sciences" as the name for the field. For example, it has been suggested that the American Chemical Society change its name to the "Society for Molecular Sciences and Engineering."[26] The Federation of European Chemical Societies changed its name in 2004 to the European Association for Chemical and Molecular Sciences. The broader name molecular sciences (MS) covers a larger part of the two supersciences—biomolecular sciences and material sciences—than chemistry does on its own.

Some chemists, such as the editor of *Chemical Innovation,* are worried about the future of chemistry as a discipline: "Chemistry as a subject is facing difficult times, and we chemists are the only people who can do anything about it. [...] If we don't do anything,

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19. Graedel, T. (1999) "Green Chemistry in an Industrial Ecology Context" *Green Chemistry* 1:G126-G128.
20. Anastas, P.T.; Warner, J. (1998) *Green Chemistry: Theory and Practice.* Oxford: Oxford University Press.
21. Mestres, R. (2004) "A Brief Structured View of Green Chemistry Issues" *Green Chemistry* 6:G10-G12. 22 Sjöström, J. (2006) "Green Chemistry in Perspective—Models of GC Activities and GC Policy and Knowledge Areas" *Green Chemistry,* 8(2):130-137.
23. Anastas, P. T.; Kirchhoff, M. M. (2002) "Origins, Current Status, and Future Challenges of Green Chemistry" *Accounts of Chemical Research* 35(9):686-694.
24. vide supra, reference 4, p. 152.
25. Nye, M. J. (1993) *From Chemical Philosophy to Theoretical Chemistry—Dynamics of Matter and Dynamics of Disciplines,* 1800–1950. Berkeley: University of California Press, p. 30.
26 Baum, R.M. (2004) "A Radical Notion" *Chemical & Engineering News* 82(45):5; Ritter, S.K. (2004) "Redefining Chemistry" *Chemical & Engineering News* 82(48):31.

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we'll be extinct in a generation."[27] However, other chemists instead emphasize the need for classical chemical knowledge in the broader and even more heterogeneous field of MS: "As the borders between scientific disciplines blur (a process that will only continue), fundamental chemistry skills such as synthesis and analysis will be crucial for the interdisciplinary subjects that emerge."[28]

27. Birkett, D. (2001) "Yuletide, Chemical Warfare, and Essential Micronutrients" *Chemical Innovation* 31(12):IBC.
28. Editorial (2001) "A Discipline Buried by Success" *Nature* 411:399.

With increasing interaction between the classical sciences and also between science and society, the meta-molecular fields discussed in this article are needed to give perspective and guidance to and about the practitioners and teachers of the molecular sciences. It is time to redefine ourselves as (meta) molecularists.

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