Chemistry education fostering creativity in the digital era

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Abstract: Renewing undergraduate education in the chemical sciences to foster creativity using research, visualization and connectivity resources has substantial benefits, but requires changes in the curriculum and teaching methodology as well as in conventional university teaching and academic human resource policies.

1. Introduction

Numerous problems affect today's science and technology education across the world, including the declining number of students enrolling in science and technology, [1] the unsatisfactory status of education in solar energy, [2] the declining interest in an academic career of PhD students in the life sciences, chemistry, physics, engineering and computer science, [3] the difficulty in communicating science to the public, [4] and, in chemistry, the declining share of public spending on research in the chemical sciences when compared to other disciplines. [5]

Industries relying on science, technology and engineering suffer from "a skill crisis" with companies "across all branches struggling to recruit new entrants into technical and research roles" while schools and universities are reported to find it difficult to interest young people in studying science, technology and engineering subjects.

In 2010, the percentage of PhD chemistry students in the U.S. interested in an academic career was found to be lowest (60%) amongst all scientific disciplines, and halved to 30% after three years of doctorate.^[3]

A recent survey of a representative sample of chemistry professionals from academia and industry found that "chemistry has an image problem", [6] with 78 percent of the sample believing that the decline in chemistry students was attributable to "chemistry's perceived lack of 'newsworthy' innovations compared to other sciences". [7]

Renewing undergraduate education in the chemical sciences to foster creativity using recent research findings and the practice

of visualization has substantial benefits, but requires changes in the curriculum and teaching methodologies as well as in teaching and academic human resource policies at universities.

These changes, we argue in this study, are key to tackle the chemistry "image problem" mentioned above, [6] increasing the number of students willing to learn chemistry across the world, and unleashing the full innovation potential of chemistry, especially with regard to its role in solving the global (and related) energy and environmental crises. [8]

Pointing to fundamental changes in the way chemical research is practiced ("a departure from past experience"), knowledge production in chemistry over the 20 years from 1990 through 2009 recorded rapid growth, which cannot be explained by any of the measurable input variables including financial expenditure. [9]

This shift in the practice of research in chemistry has been due to the fact that chemical research in the digital era has become multidisciplinary and collaborative beyond national borders. Collaboration with scholars from other disciplines and often from other countries has become the norm, with most research papers today including authors from widely different scientific backgrounds, including human sciences.

Yet, as the former chair of the committee on chemistry education at International Union of Pure and Applied Chemistry (IUPAC)^[10] has lately emphasized "many of our textbooks and teaching approaches are stuck in the past and haven't changed much in the past 30-50 years. So much of the growth of chemical knowledge in cutting edge areas that cross disciplines is therefore lost to our students".^[11]

2. Research-enhanced education

Findings of fifty years of research in chemistry education, [12] suggest a number of changes in undergraduate chemistry curricula, educational materials and teaching methodologies. Yet, to quote the same leading scholar in chemistry education research writing in 2014, change in the practice of chemistry education has been "glacially slow". [13]

To teach the fundamental concepts of today's green natural product extraction Professor Farid Chemat at the University of Avignon, France, uses state of the art microwave hydrodiffusion and gravity technology to extract essential oils, vitamins, colors, biophenol antioxidants and numerous other bioproducts (Figure 1). [14]

In the laboratory, students compare the new method with older processes such as conventional hydrodistillation or Soxhlet extraction with *n*-hexane. "Education in this way", Chemat suggests, "materializes the concepts and principles of green chemistry and engineering, whereas further education in the classroom instructs tomorrow's chemistry practitioners on the

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need to effectively communicate the benefits of a greener product for the final consumer". $^{[14]}$







Figure 1. Practical work on green and conventional extraction techniques for Master students at Avignon University. [Reproduced from Ref.14, with kind permission].

In the U.S., the students in organic chemistry at Marshall University taught by Professor Kenneth J. O'Connor since 2013 use a new solid palladium catalyst to practice and more closely understand today's green synthetic organic chemistry. [15] The catalyst successfully mediates the main carbon-carbon cross-coupling reactions and is also an highly selective hydrogenation mediator affording the saturation of a wide variety of alkenes and alkynes with experimental yields ranging from 60-95% under ultra-mild conditions.

In detail, students are given the catalyst and one of three alkenes (dimethyl fumarate, trans-cinnamic acid and methyl trans-cinnamate) and are requested to carry out the hydrogenation reaction in 2-Methyltetrahydrofuran under H_2 balloon conditions (Figure 2).

2-Methyltetrahydrofuran, they are further taught, is a green solvent^[16] whose boiling point, higher than commonly employed methanol, would also lead to higher solvent recovery on an industrial level.

With a single experiment, students learn the use of spectroscopy methods coupled to qualitative TLC to follow the course of a reaction, and are taught green chemistry principles by calculating the green chemistry metrics E factor and assessing the atom economy of the reaction (Table 1).

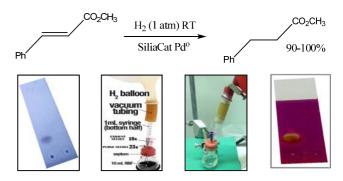


Figure 2. The reaction scheme (*top*) for the hydrogenation of methyl *trans*-cinnamate mediated by Silia*Cat* Pd(0). The progress of the reaction is determined by TLC (*bottom*). At the end of the experiment, the solution is filtered and the solvent evaporated to yield the saturated ester or carboxylic acid. Spectroscopy is used to confirm the product's structure by comparing the NMR and IR taken to the literature spectra. [Image courtesy of Prof. K. O'Connor, Marshall University].

Table 1. Questions to organic chemistry students at Marshall University after laboratory hydrogenation led by Professor Kenneth J. O'Connor.^[15]

- 1. How did you know that your reaction went to completion?
- 2. Assuming your yield is not 100%, where do you think the biggest losses occurred in this experiment?
- 3. What is the mechanism typically proposed for the hydrogenation of an alkene using a transition metal catalyst?
- 4. Which reagent has the largest effect on the E factor in this experiment? If this reaction were conducted in an industrial setting where solvent recovery was much higher than in your experiment, what would happen to the E factor?
- 5. How can you determine spectroscopically that the reaction has gone to completion after isolating your product?
- 6. Calculate the yield, atom economy, and E factor for your reaction. Explain what these values mean for each calculation.

3. Visualization-enhanced education

"Now I am going to look at molecules in a different way. There is no sharp distinction between symmetry and no symmetry – there are a lot of levels in the middle" commented in 2010 a chemistry high-school teacher in Israel after using an online visualization tool (the Molecular Symmetry Online website, http://telem.openu.ac.il/symmetry, Figure 3) to view molecules and their symmetry elements in three-dimensions.

Along with a a group of experienced chemistry teachers, the educator performed online calculations of continuous symmetry measure (CSM, a number between zero and 100 providing a quantitative description of the distance a particular structure has from perfect symmetry)^[18] with emphasis on the chemistry, rather than on the mathematics.^[17]

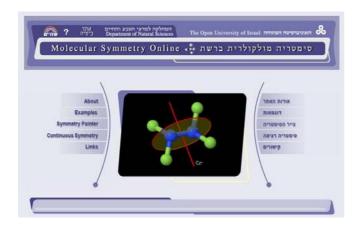


Figure 3. Home page of the Molecular Symmetry Online website managed by The Open University of Israel at: http://telem.openu.ac.il/symmetry.

The team discovered that the visualization tool expanded their view of the three-dimensional structure of molecules and improved their understanding of molecular internal motion (vibration and rotation) whereas even a very basic knowledge of symmetry and continuous symmetry opened up new ways of thinking about and looking at molecules.

Suggesting that their experience could shed light on curriculum choices for teachers' education, Tuvia-Arad and Blonder concluded that "results indicate that highly advanced content can influence the way teachers think, understand, and eventually teach." [17]

The chemical methodology guiding the *creation* of new and useful substances is indeed based based on visualization and association of chemical building blocks, most notably atoms and molecules.^[19]

Following the introduction of quantum mechanics in the 1920s, said methodology been expanded by the use of incommensurable theories resulting from the interplay of quantum mechanics and heuristic chemical concepts, resulting in rules and models, such as those concerning chemical reactions based on rearrangement of electron pairs as bonds are made and broken, of great utility as predictive tools.^[19]

In the digital era visualization, transforming data into graphical structures, can become computer-supported and interactive. [20] The aim of producing visual representations of data, though, remains unvaried: to amplify the understanding of the phenomona being studied as "understanding often comes from seeing". [21]

"Computer-supported and not computer-based",^[21] suggests Valle, since "visualization does not speak to machines, it speaks to humans" and is "useless without human pattern recognition and without our openness to creative and serendipitous discoveries".^[21] According to the same science visualization scholar, the main obstacle on the path to a more generalized use of visualization in (quantum) chemistry would be

"considering visualization a way to produce nice images only and not a data understanding process". [21]

It is this visualization process that explains for example the success of the reaction mechanism approach to teach and learn organic chemistry first proposed by Wentland in the early 1990s, [22] and lately streamlined and expanded by Ogilvie and Flynn, [23] along with other organic chemistry professors in Canada. [24]

"This approach leads to a greater understanding and appreciation of organic chemistry as attested by the many students from several universities who have taken my courses" [22] wrote Wentland in 1994 in *The Journal of Chemical Education*.

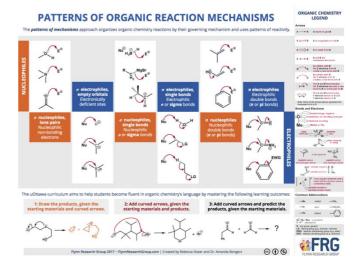


Figure 4. The patterns of mechanisms approach developed by Flynn, Ogilvie and co-workers at the University of Ottawa organizes organic chemistry reactions by their governing mechanism and uses patterns of reactivity [Image reproduced from www.flynnresearchgroup.com/research, with kind permission].

This approach has been successfully used since early 2012 at the University of Ottawa. Recognizing reaction patterns based on electron flow promotes understanding and, once again, allows students to predict the outcomes of reactions they do *not* yet know. In this way, students do not have to memorize a large set of reactions while becoming, to quote Professor Flynn, "fluent in organic chemistry's language" (Figure 4).^[25]

Rather than organizing the discipline around structure, the discipline gets organized around reactivity, progressing from simple reactions, such as that between acid and base, to more complex ones. [23] Before students learned any reaction, first the electron-pushing formalism mechanisms and and the principles of reaction mechanisms are taught in the first semester. Second, reactions arranged based on the pattern of their governing mechanism, rather than by functional group, are taught in the first and second semester of organic chemistry. [23]

The mechanisms are taught in a gradient of difficulty by teaching first the mechanistically most simple reactions and then the

more comples ones. The team authored a textbook^[24] organized around the principles of reactivity, rather than on structures (alkanes, alkenes, alkynes and so on) including as a visualization tool a software (ChemWare) allowing students to visualize the dynamic mechanism of the main organic reaction mechanisms taught.

Studying the impact of the electron flow, mechanistic approach to teaching organic chemistry in action by analysing the exam results at the University, Flynn and Featherson lately found that students actually attributed the correct meaning of electron-movement and bond formation/breakage to the curved arrows used in the formalism. [26]

4. Connectivity-enhanced education

Engaging students in learning in the digital era requires that professors find new ways to incorporate into lectures and discussion held in the classroom the information and knowledge that students "acquire outside class in their digital lives". [27]

Digital connectivity thereby becomes a key aspect of today's teaching, as well as of carrying out research, which explains why most today's leading chemistry scholars operate updated personal websites and make systematica use of the main social networks: not to increase their reputation, but rather to get feedback and start new personal interactions and collaborations.

Indeed, trying to explain the dramatic growth in knowledge production in chemistry occurred between 1990 and 2009, one of the hypotheses made by Rosenbloom and co-workers was that spread of automatic laboratory data collection and analysis using personal computers and the internet. [9] In other words, new information and communication technology would be responsible for the increase in the productivity of academic chemistry.

Further supporting this explanation, we add that a study of the content of this new chemistry research would reveal that most of said scholarly output has become multidisciplinary, with the boundaries that defined the old domains of chemistry teaching and research, reflected in the scholarly journals in "inorganic chemistry", "physical chemistry", and "organic chemistry", having broken down.^[28]

Today's research in chemistry is interdisciplinary in nature because in the last decade of the 20th century, facilitated by the emerging Internet, World Wide Web and electronic mail technologies, research chemists started to collaborate not only with colleagues in the former chemistry departments but also with scholars from other faculties, including biology, physics, computer science, engineering, medicine, archaeology, cultural heritage and many other formerly strictly separated disciplines.

Do today's students pervasively use smartphones and their applications (apps) even during classes? Chemistry educators in Singapore, then, lately developed a method using social media Instagram and Snapchat apps for laboratory teaching purposes

to strengthen the concepts learned during the curriculum and facilitate learning. $^{\left[29\right] }$

A public account was created for both Instagram and Snapchat to facilitate the sharing of the real-time content with the students. Different images and videos of the week's experiment were captured and uploaded onto Snapchat first. The instructor adds a caption to explain the main takeaway in the "snap", or pose a question for the students to think about. Similary, videos and pictures are uploaded onto the Instagram feed.

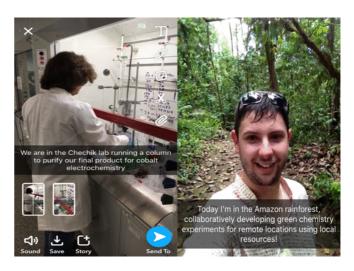


Figure 5. A Snapchat video screenshot of Prof. G. Hurst, York University, demonstrating how to run a column in a research laboratory and how the instructor has provided students a glimpse into their professional life. [Image reproduced from Ref.30. with kind permission].

The educators discovered that through instant sharing of images and videos on both platforms, information could be shared and disseminated to the students much more quickly, especially when the instructors or the technical assistants were not able to attend to every student's question at the same time. Uploaded content helped for example to emphasize the correct execution of a certain procedural step that has been done incorrectly by previous groups of students, so that other students could learn and avoid to commit the same mistakes.

The mid-semester survey module of 75 students (response rate: 72%) conducted five weeks after Instagram and Snapchat were incorporated into the, clearly showed that the majority of the students felt that the applications were helpful to them in several ways. For example, the images and videos uploaded helped the students to increase their retention of chemistry knowledge (88%), increased their understanding of both theoretical and practical aspects after each experiment (80%), and allowed them to correct their mistakes (89%).

Similarly, Hurst in Britain sends undergraduate students studying chemistry, biochemistry, and natural sciences students a blend of annotated pictures and videos on Snapchat (Figure 5) to allow them to to contextualize subject knowledge in the real world, and enhance student engagement with chemistry, and

provide an insight into research environments and life as an academic in chemistry. $^{\left[30\right] }$

Images and videos were shared using an account followed by 140 students. Survey of the students (43% response rate) showed overwhelmingly agreement (4.32/5.00): students feel more engaged with chemistry when using the social media app, which was found by most students also a most useful tool to contextualize knowledge and understand how chemistry can be applied to affect daily life.^[30]

5. Shaping scholars, and not researchers

Following Lévy-Leblond's insight into the role of contemporary science in culture, [31] the aim of today's and tomorrow's chemistry education should be that to shape chemistry scholars (and not specialized researchers) capable to carry out multidisciplinary research, and subsequently to teach the subject to digital native students.

This requires several key changes to previous ways of training researchers. First, we need to train new professional scientists providing them with a basic understanding of the history of science - and above all of chemistry, as well as of philosophy, sociology and the economics of science. "The tasks they are currently faced with in their profession as well as the social responsibilities they can no longer avoid demand that... we cannot go on behaving as if science...could be taught independently of its history". [31]

Second, aware of evidence from chemistry education research on meaningful learning,^[32] chemistry professors will assess students' prior knowledge and each time teach topics being explicit about what the new knowledge is to be used for (namely to explain to students *why* they are learning a topic).^[31] Furthermore, since effective teaching is student-centered, the intructor will ask questions both during and at the end of each class to prompt reflection on what students have learned and to promote learning through discussion.

Third, chemistry educators will convey to students a clear and better understanding aware of the unique chemistry methodology to *create* new and useful substances based on mental visualization and association of chemical building blocks for substances originating the cornucopia of new man-made substances which benefit society at large.^[19]

Fourth, to face the chemists' difficulty in communicating with the general public (worsened by limited chemical knowledge of ordinary people), [33] educators will integrate science communication training into dedicated lectures focusing on how actively and effectively communicating about their work the general public. As suggested by Steinman neurology and biology and co-workers at Stanford University, science communication is "a difficult skill that many practicing scientists lack, likely due to the combination of increased specialization over time and the absence of formal training in science communication". [34]

A most instructive excersise will be that suggested by Hart and Chappell, namely that along with every scientific article, a public abstract in plain English (100 words or less, using no jargon) is posted on the Internet for the public as well as for journalists.^[35]

Fifth, chemistry educators will teach the basics and the tools of open science, offering a critical overview of the changes occurred in knowledge creation (research and scientific collaboration) and distribution (and scholarly publishing) induced by the Internet since the late 1990s, [36], including the recent remergence of preprints in chemistry. [37]

Mario Pagliaro is a chemistry and energy scholar based in Sicily, at Italy's Research Council, where he has worked for the last 20 years after studying and working in Italy, the Netherlands and in Israel. Developed in cooperation with leading scholars based in over 20 countries, the outcomes of his research group's work in chemistry, solar energy and the bioeconomy are reported in over 200 frequently cited research papers. Author or co-author of 21 books, including *Solar*



Hydrogen and Helionomics, Dr. Pagliaro has been often cited for his excellence in teaching. Following the Quality College of the CNR (1998-2004), he helped to establish Sicily's Solar Pole (2008-2017), two lively educational and research centres, and today ranks amongst Italy's most cited scientists in nanotechnology and materials chemistry. In recognition of his "significant contributions to the chemical sciences", in 2014 he was designed Fellow of the Royal Society of Chemistry. He regularly organizes conferences and gives courses and seminars on the topics of his research. He is among the invited plenary lecturers at XX International Sol-Gel Conference, the leading sol-gel materials science and technology conference, celebrating its 20th anniversary in St Petersburg, Russia, on August 2019.

6. Learning organisations, rewarding teaching

If universities wish to support a professional teaching approach that mirrors the approach for research, then, "there has to be an acceptance that teachers must become reflective practitioners, and an intention by university management to create the conditions that foster and reward this rather different approach". [38]

Laurillard has aptly argumented that academics "work to the system in which they find themselves". [38] Hence, universities willing to promote a highly professional approach to teaching among faculties will need to deploy a career and financial reward system targeting both research and teaching, in place of that so far largely dominating across the world which mostly rewards research achievements only.

Studying teaching award-winning faculties in a researchintensive U.S. university, scholars in higher education lately found that the main suggestion of said leading faculty member educators to their universities is to create teaching centers to provide training, mentorship, professional development, and opportunities for collaboration around teaching.^[39]

This brings us again to Laurillard's call for the need of teachers to become "reflective practitioners". The percentage of chemistry professors and educators who received formal training in teaching is low in most world's countries, and while this could be an acceptable feature of universities of the past, training a low number of chemistry students, this is no longer the case in today's academic organisations in which a significantly larger number of undergraduate students attend different chemistry subjects as part of academic multidisciplinary courses significantly different from the past.

Finally, teaching in an organisation (the university seen as a system) whose purpose is defined from the customer's (*i.e.*, student's) perspective to 'provide me with all the facilities and help I need to achieve a positive outcome from my time at your university', [41] educators will shape programmes and teaching methodologies around what matters to students, including to gain a systemic understanding of how to continue to make improvements.



Figure 6. Picture from a lecture on natural product extration of Professor F. Chemat at the University of Avignon, 2009. [Image courtesy of Avignon University. The whole lecture (in French) is available online at: goo.gl/PYSVsd].

Professor Chemat, for example, in the classroom uses the old chalk and talk method of teaching (Figure 6), in a two-step learning process in which he first gives a conceptual and historical introduction of natural product extraction, and then offers the technical developments.^[14] A glance to the public recognition of his former students published online on the World Wide Web and its social networks is enough to realize how this approach is actually appreciated by Avignon's chemistry students.

Other educators use case studies to promote learning of key chemistry concepts and comprehension of their relevance to their lives, including a context-based approach to the teaching of undergraduate physical chemistry, using the context of the next generation of energy for a city using physical chemistry

principles to examine the combustion of fossil fuels (and hydrogen) compared to the use of hydrogen in fuel cells, solar photovoltaic power, and energy from a geothermal source. [42]

Students, the educators found as early as of 2005, welcome studying physical chemistry within an applied context, rapidly developing a subject knowledge whose societal relevance could now be clearly perceived.^[42]

These findings are all the more relevant as it will be the creativity of tomorrow's chemistry scholars that will play a crucial role in solving the global (and related) energy and environmental crises by developing the low cost clean electricity storage technologies mankind urgently needs to achieve the transition to renwable energy.^[43]

Eventually, the guidelines suggested by this study building on relevant previous work of chemistry education scholars, will ease the work of chemistry professors and universities seeking new ways to improve chemistry teaching and learning and make chemistry an attractive subject for the vastly number of students studying chemistry subjects in the digital era.

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Keywords: chemistry education • digital era • visualization • energy crisis • chemistry research

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PERSPECTIVE 8

Chemistry education fostering creativity in the digital era

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Reshaping chemistry education to foster creativity? Yes, but how? Using research, visualization and connectivity resources, this study suggests. Changing not only the curriculum and teaching methodology, but also the university teaching and academic human resource policies.

