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Review of *Pioneers of Quantum Chemistry*

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Pioneers of Quantum Chemistry; **ACS Symposium Series 1122**, by E. Thomas Strom and Angela K.Wilson, Eds. American Chemical Society: Washington, DC, 2013. 330 pp. ISBN 978-0841227163 (hardcover). $ 150.00 (Individual chapters downloadable for ACS members).

There is little doubt that reading books other than textbooks represents an important component of maintaining knowledge for many chemistry educators. Nonetheless, with 30 or more books a year being produced by the ACS Symposium Series alone, how can choices be made about what merits reading time? Certainly, the presentation of current research trends that might influence the chemistry taught in courses represents one metric, but there are many additional worthy books. In terms of potential teaching treasures to be mined, time spent reading history of science presents a strong possibility.

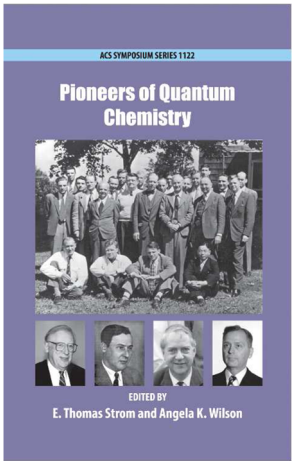
A recent article by Scheffel et al.[1] provides an important argument in support of the inclusion of historical developments of content matter in chemistry. These authors present a metastudy of the literature[2−7] and provide nine points of value for including aspects of history in teaching:

- Students gain a better understanding about "the nature of science as a social construction".
- Students may be trained in critical thinking to a greater extent.
- Knowing more history may help teachers connect chemistry to other curricular content and social contexts.
- Students may have ideas about chemistry topics that are similar to those held by scientists at some point in the historical development of our understanding.
- Historical content may afford avenues to construct "rich learning opportunities" that connect real-world experiences, historical developments, and scientific problems.
- For some students, stories from history may provide motivation for learning.
- Properly chosen stories might help students identify with scientific personalities.
- Students may learn that chemistry has long been an intellectual pursuit that plays a role in how human culture advances.
- Historical controversies in particular can help students change preconceptions about chemistry, essentially by serving as a model of how science itself changed its views.

While some of these possible influences might be more readily perceived as valuable to any given teacher than others, in total they comprise an important argument for the inclusion of the history of chemistry in chemistry classrooms.

In some ways, the idea of the atom and the manner in which science came to understand atoms and their role in chemistry represents a particularly significant example. Atoms and atomic structure are inherently abstract constructs, and students over time are bombarded with a number of models for what atoms are. It is unsurprising then that hybrid models,[8] in which students essentially pick-and-choose components of different models, have been observed among chemistry novices. It has been argued that the development of mental models of atoms represents a threshold concept for students.[9]

This context of the potential role of history in teaching and the importance of student conceptualization of atoms argues strongly for consideration of the book *Pioneers of Quantum Chemistry* to be on the bookshelf of chemistry educators. Fortunately, in many important ways, this ACS Symposium Series book does not disappoint. As is true of any symposium book, the chapters are not particularly designed to flow into each other, but there are pieces of interesting information throughout. In many cases the narrative shifts between the personalities who worked on quantum chemical ideas and the description of the ideas themselves. As a result, the connections to possible teaching benefits present themselves on a regular basis. One of the key advantages of this particular collection of historical articles lies in the fact that several of the authors were present during the developments that are described, or had personal correspondences with key figures in the development of quantum chemistry.



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It is dangerous to encapsulate the presentations of each chapter in a few sentences, but for a collection such as present in this book, the potential for a tedious read seems to be outweighed by the advantage of getting a glimpse of the content. The book begins with a chapter titled "Three Millennia of Atoms and Molecules". This chapter sets the

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stage well for the entire book by tracing the historical origins of quantum chemistry to the dawn of human intellectual grappling with the nature of matter. The chapter is broadly inclusive of a large number of concepts that were important in the long-term development of atomistic thinking about nature, as well as noting competing concepts along the way. When it arrives at the developments of the mid-20th century in quantum chemistry, the chapter authors leverage their personal experience as researchers in the field to provide firsthand accounts with some rare historical insights that have fortunately been captured in this account. The second chapter, "Pioneering Quantum Chemistry in Concert with Experiment", by Hargittal includes both key conceptual developments for the development of quantum chemistry and interesting historical stories. In particular, it includes a description of how governmental directives about the concept of resonance in what was at the time the Soviet Union influenced the development of quantum chemistry in that country. This story is visited briefly in other chapters as well, and shows how political prerogatives were directly interjected into the progress of scientific understanding in a more culturally combative time.

Resonance theory, as an important step in the development of the quantum understanding of bonding, plays the leading role in Chapter 3, "George W. Wheland: Forgotten Pioneer of Resonance Theory". This chapter takes a more biographic account of the development of resonance as a concept, particularly as applied in organic chemistry. Nonetheless, the key conceptual underpinnings, and how the scientific community came to understand them, are fundamental to the presentation. Chapter 4 proceeds to the "The Free-Electron Model" and argues that the ability to connect the particle in a box model of quantum mechanics to conjugated bonding systems represented an important advance for the utility of quantum chemistry in an era prior to high computational powers afforded by the development of the computer. For teachers of chemistry, this chapter makes specific connections to the importance of this development for pedagogy.

Chapter 5, "Michael J. S. Dewer: A Model Iconoclast", returns to a more encompassing biographical approach to the development of quantum chemistry, particularly reasoning with orbitals. Perhaps more than other chapters, this one includes amusing personal anecdotes about the personality of Dewer in addition to the science to which he contributed. Chapter 6 continues the biographical approach with "H. C. Longuet-Higgins: The Man and His Science". While Longuet-Higgins contributed important research to MO theory, this chapter also presents his contributions to more varied theoretical pursuits, including statistical mechanics. From the perspective of MO theory, the chapter provides several examples of how the concepts were refined over time.

The importance of the relationship between computing and quantum chemistry steps to the forefront starting in Chapter 7, "The Golden Years at LMSS and IBM San Jose". The role of the Laboratory of Molecular Structure and Spectra (LMSS) at the University of Chicago, which is noted in previous chapters, is specifically highlighted in this chapter. Contributions of R. S. Mulliken and C. C. J. Roothan while at the LMSS provide one key component of this chapter, and those of Enrico Clementi at IBM in San Jose organize the other component. While centered on the contributions of these three scientists, the ability to cast quantum chemistry problems in terms that could take advantage of emerging computer power is the conceptual theme that their stories allow to be told. Chapter 8, "Quantum Chemistry Program Exchange, Facilitator of Theoretical and Computational Chemistry in Pre-Internet History", continues the discussion of computational power, but with a more software emphasis. Capturing the collaborative nature of computer code development in the 1970s and 1980s provides an interesting story that seems prescient for modern day efforts among a segment of scientists toward open access publishing.

Chapter 9, "Molecular Orbital Theory for Organic Chemists", returns with a more focused approach to a topic that was previously mentioned in several locations in the book: Hückel theory. It argues the ability of quantum chemistry to address aromaticity with a relatively simple model played an important role in how theoretical concepts diffused into other areas of chemistry, principally organic. The development of HOMO−LUMO reasoning is also featured in this chapter. Finally, in Chapter 10, "John Pople: The Man and His Science", the biographical account is told of Pople and his efforts to generate practical capabilities for quantum chemistry outside the community of its developers. In many ways, this is a fitting final chapter, in that making quantum calculations more readily done by chemists outside of a core of theory researchers represents a key transition to the next stage of its development as a field.

In total, *Pioneers of Quantum Chemistry* presents a number of potentially useful concepts for the chemistry educator. When one thinks about the nine previously mentioned categories for inclusion of history in the teaching of chemistry, the book provides several connections. First, the stories of personalities involved in the advancement of quantum chemistry abound in this book, and such stories can allow students to identify with scientists and may improve motivations for learning. Because of the interconnection of many of the characters and anecdotes about their interactions, these biographical accounts also serve as examples of the social construction of scientific knowledge. Stories of controversies in understanding bonding in terms of resonance, for example, could inform the inclusion of information about how models in science change over time. Finally, there are plenty of topics that show how the application of quantum chemical ideas developed and these could form the basis for critical thinking exercises and the construction of multifaceted problems for students. Within the context of these avenues for the inclusion of historical treatments in the teaching of science, *Pioneers of Quantum Chemistry* has many positive attributes. For readers with less time, downloading the first chapter (perhaps with one of the downloads ACS members obtain with their membership) with its excellent tracing of the concepts of atoms and bonding throughout human intellectual history is worth a look.

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Notes

The authors declare no competing financial interest.

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