

Book Review

E. Thomas Strom & Angela K. Wilson (eds.): *Pioneers of Quantum Chemistry* (ACS Symposium Series, vol. 1122), Washington, DC: American Chemical Society, 2013, v+330 pp. [ISBN: 9780841227163]

by Kostas Gavroglu

Reading books like this volume, a professional historian or philosopher of chemistry poses, I am sure, the question of what the net effect of so many years of scholarship in history and philosophy of chemistry has been on practicing chemists, and especially, on those who are interested in and write about the history of various subjects of chemistry. And, if one tries to examine this question through the essays of this otherwise informative book about the developments in quantum chemistry, then the answer is that works in the history and philosophy of chemistry have had almost no effect on the professional chemists, and have left them rather indifferent. This is not a criticism neither against the chemists nor against the historians and philosophers of chemistry, but an observation which comes out after reading the present book. Unfortunately, reading other similar books in chemistry or physics, this assessment remains the same.

The question is, of course, not whether chemists should rely on historians for the validation of facts, nor is it the case that they should rely on philosophers for the clarifications of concepts. The serious problem is not whether some such works would be cited by the chemists who write historical pieces, but the lack of involvement and the lack of constructive criticism by the chemists on the various issues articulated by historians and philosophers of chemistry – such as reductionism, the relative independence of quantum chemistry with respect to physics and mathematics, the character of semi-empirical theories, the ways different styles of thinking can be traced in the development of quantum chemistry, *etc.* It is a pity that even though many of the authors of this volume had an opportunity to comment or engage with a number of historiographical and philosophical issues, almost all of them did not. Of course, it may be the case, that many chemists find such aspects of the scholarship produced by historians and philosophers of chemistry superfluous, uninteresting, useless, or plainly trivial. Still, it would have been aca-

demically much more challenging to exchange views on these issues than remain silent.

Another thing that especially historians are rather sensitive to, and this volume would have been an excellent place to do it, is to discuss failures in quantum chemistry and try to understand them in their proper contexts. The great majority of scientists (chemists, of course, included) are interested in narrating the lasting contributions, the peaks of the various developments. But much of the everyday work by scientists ends up in failures. Predictions that did not realize, calculations which turned out to be wrong, hypotheses that were not justified, approximations that underestimated or overestimated various factors, *etc.* This is neither fraudulent science nor bad science, but science as it is practiced by the protagonists as well as the rank and file. And it would have been very interesting to read the views of the authors of this volume about the failures in quantum chemistry, since these have been an integral part of their science. Here, as elsewhere, the common thread and the overall picture is one of yet another success story of chemistry. A success, however, whose history had been infested with failures and dead ends. It is a pity that we get only some very partial glimpses of these dead ends.

Historians and philosophers of chemistry have, also, developed a number of techniques that may be useful in such undertakings. One of these techniques is to look carefully at the archival material left by the person under examination and try to assess most of what has been published in the context of more private thoughts exchanged with other colleagues in correspondence, or jotted down in notebooks. Most of the authors of these essays write their narratives as if they are unaware of such a way of tackling the work of their subject.

Klaus Ruedenberg and Eugen Schwarz give a compact yet self-contained narrative about the ideas concerning the atomic constitution of matter and the ways these have theoretically been dealt with, emphasizing that their 'perspective is that of active researchers in theoretical chemistry'. Istvan Hargittai, through a number of personal reminiscences relates the relations of the various theoretical schemata in quantum chemistry with experiment. Paul Bagus compares the work in two research centers (the Laboratory of Molecular Structure and Spectra (LMSS) at the University of Chicago and the Large Scale Scientific Computations Department at the IBM Research Laboratory in San Jose, California), one on theoretical and the other on computational chemistry, points out synergies between the researchers, and discusses the decisive role of the centers in the distribution of the various computer programs in order to calculate electronic structures. Donal Boyd's article is a narrative about the Quantum Chemistry Program Exchange based at the University of Indiana, which for thirty years played an important role when chemists and software experts would exchange algorithms at an international

level to make the calculations feasible that seemed impossible until about the beginning of the 1960s. Andrew Streitwieser discusses molecular orbital theory for organic chemists mainly based on Erich Hückel's work and to a lesser degree that of Charles Coulson. William Jensen outlines the historical development of the free-electron model, has pictures of three dimensional pen and pencil models that were very useful before the advent of the computers, emphasizing its continuing pedagogical significance. Four articles examine closely the lives of particularly significant figures in the development of quantum chemistry: E. Thomas Strom, one of the editors of the volume who has served as president of the ACS section on history, has written a rather interesting short biography of George W. Wheland, by taking advantage of his correspondence as well as the secondary literature on him. Wheland, one of the most active chemists in developing Pauling's resonance theory for the chemical bond and with important contributions in orbital theory, was a person of amazing inquisitive skills concerning the character of resonance itself, that is concerning its ontological status. Eamonn Healy discusses a number of issues concerning the developments in quantum chemistry through the work of Michael Dewar. Weston Thatcher Borden talks about Longuet-Higgins, and with a 'what if...' view concerning Nobel prizes. Janet Del Bene examines the life and work of John Pople, who was absolutely decisive in making computational chemistry something practical for many chemists by devising computer programs and algorithms.

Overall this is a particularly useful volume, with an immense amount of information, some of which was unknown to this reviewer. At the same time, it is a book which should force all of us – historians, philosophers, practicing scientists – to (re)assess the perennial question concerning the characteristics of our audiences and the effects of the scholarship produced by one such group on the scholarship produced by the others.

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