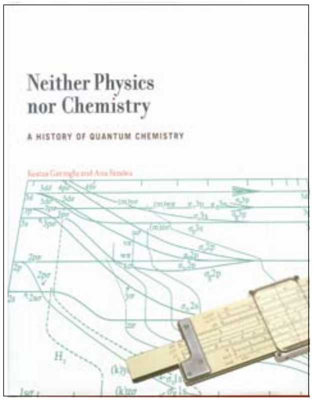


Neither Physics nor Chemistry: A History of Quantum Chemistry. Kostas Gavroglu and Ana Simões. The MIT Press, 55 Hayward Street, Cambridge, MA 02142, USA. 2012. xiv + 351 pp. Price not mentioned.

Dirac's infamous 1929 statement, 'The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble', is considered by many to be an epitome of reductionism. About 50 years later, Edgar Bright Wilson summed up his article (*Pure Appl. Chem.*, 1976, **47**, 41) titled 'Fifty years of quantum chemistry' as follows: 'Chemistry has a method of making progress which is uniquely its own and which is not understood or appreciated by non-chemists. Our concepts are often ill-defined, our rules and principles full of exceptions, and our reasoning frequently perilously near being circular. Nevertheless, combining every theoretical argument available, however shaky, with experiments of many kinds, chemists have built up one of the great intellectual domains of mankind and have acquired great power over nature, for good and for ill. My guess is that they will continue to work in this way and that any new results and methods from quantum theory will be built into the structure just as the old ones, errors and all, have been.'

In the 50 years timespan bridging Dirac's and Wilson's statements a relatively quiet revolution, by physics standards, now called quantum chemistry has happened. In this book, Gavroglu and Simões trace the developments of quantum chemistry through its various avatars – from being physics, chemistry, applied mathematics, to finally a computational science. Today, undeniably and appropriately, quantum chemistry is in a superposition of all these avatars. However, as the intriguing title of the book suggests, the journey was anything but smooth. Nicholas Turro's words (21st C, issue 3.4) 'The emergence of quantum chemistry warns us that no matter how bizarre a scientific claim may be, or how remote from ordinary experience, it can still eventually be accepted and embraced by the relevant community,' is a mild indicator of how tortuous the journey must have been! In this context, an article (*Logic Philos. Sci.*, 2008, **6**, 3) by Hettema (a theoretical chemist turned unpaid philosopher working in an IT company) titled 'Is quantum chemistry a degenerating research programme?', wherein he takes on the philosopher Andrea Woody's claim that it is so, is worth a read.

The twists and turns are nicely narrated by interwoven stories of individuals and groups, their single-minded pursuit, the glorious debates, and the obstinate viewpoints which have contributed enormously towards establishing quantum chemistry as an integral part of modern chemistry. For example, the debates and exchanges between Pauling and Coulson on the notion of resonance structures makes for an interesting and illuminating reading. The constant jostling around of ideas involving Heitler, London, Pauling, Hund, Slater, Van Vleck and Mulliken with the 'Americans' versus the 'Germans' theme gives a glimpse of the early heady days of quantum chemistry. At the same time, the important contributions of the British school are described in great detail in the third chapter. Key contributions by Lennard-Jones, Hartree, Coulson and Longuet-Higgins and their overarching philosophy of obtaining useful but consistent approximations using mathematical techniques provide another vantage point to appreciate the challenges involved. The brave attempts to understand bonding in large molecules by the French group of Daudel and Pullman and the inevitable dawn of the large-scale *ab initio* computational era are described in an abridged form in the penultimate chapter. Here one also senses the exasperation, of some, about the computers leading to a potential alienation from the more traditional ways of describing and understanding chemistry. Today, the initial exasperations have given way to the wide middle ground wherein the digital computer is intelligently used as a research instrument, as Ransil expected back in 1960. Yet, the fear of the 'black-box' blunting one's critical faculties continues to haunt many, and appropriately so if I may add. Thus, it is not surprising that a quarter of a century after Ransil and others worried about this issue, Fritz Schaefer in the preface to his book (*Quantum Chemistry: The Development of Ab Initio Methods in Molecular Electronic Structure Theory*, Dover, 1984) warns 'Nevertheless, one must concede that there are great perils associated with the application of *ab initio* methods to chemical problems...it is very easy to submit a deck of computer cards to a standard quantum mechanical program such as GAUSSIAN 70 and receive as output totally meaningless results. In fact, it is probably not an exaggeration to state that there are literally hundreds of such error-ridden calculations which have actually been published in the chemical literature.' The notion of 'intelligent' use of computers is aptly brought out in the case of the development of the Pariser–Parr–Pople semiempirical method. Pariser, doing calculations on a mechanical desk calculator, had to invoke his experimental insights to come up with reasonable parameters! Even today this acute sense of experiments is what distinguishes a run-of-the-mill calculation from an inspired one. Clearly, Löwdin seemed to have such a vision in terms of 'meaningful semiempirical theories' – quantum chemists boasting about conceptual advances rather than simply bragging about the size of the basis and the speed of the computer.

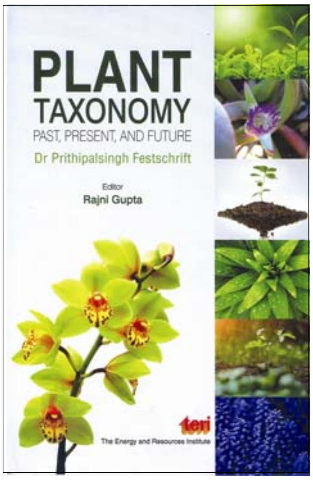
The various chapters in the book also bring forth a central issue, one that is particularly close to the chemists' heart. Can the intuitive visualization models of the chemists coexist peacefully along with the more rigorous (obviously correct and 'abstract') viewpoint of electronic structure theory? Thus, Mulliken already thought that Pauling's the nature of a chemical bond was an oversimplification. Indeed later on Mulliken said, 'I believe the chemical bond is not so simple as some people seem to think' – one of the most classic understatements of all time, according to Coulson (*Rev. Mod. Phys.*, 1966, **32**, 170). Coulson himself believed that a bond is 'no more real than the square root of –1!' Yet, in this new millennium and the age of supercomputers, we continue to use the orbitals, resonance structures, local descriptors of reactivity and the 'magical arrows' which gently guide the electrons from one bond to another. Perhaps it has to do with the insights offered by Wilson on the method in the madness of chemists! Non-chemists are not privy to such higher forms of thought and creativity. Thus, when one mixes up molecular orbital and valence bond arguments with impunity there are no voices of dissent for a simple reason – the arguments explain the experimental results. Whatever the reasons might be, quantum chemists still have this great challenge of finding and explaining, in McWeeny's words, the 'primitive patterns of understanding'.

Another important point that the authors make in this book is about the differences in the outlook of the German and American schools which led to the dominance of the latter in the development of the field. Thus, after their key initial contributions, Heitler, London, Hund, Húckel and Born could not carry on in the long run. Whereas the likes of Lewis, Pauling, Mulliken, Van Vleck and Slater helped establish a strong school of quantum chemistry that continues to date. The key difference, as the authors put it, is that in the United States whether a scientist was defined as a chemist or a physicist was just a matter of chance, personal preference, or of institutional affiliation. Consequently, interdisciplinarity was the rule rather then the exception, in stark contrast to the then German academia. This is also evident from the establishment of the Swedish school in Uppsala, thanks to the strong personality of Löwdin and his interdisciplinary outlook. There is an important and clear message here to anyone who is rather dismissive of fields, and even approaches, other than his or her own!

This is a carefully written book, albeit density functionals have been shortchanged, and will be a joy to anyone interested in the history of this unique field of research. Perhaps it can be a bit daunting for others. To them, I suggest starting from the last chapter. Although this advice is like asking someone to start from the last chapter of a Sherlock Holmes' novel, thus taking that element of the unexpected away, it may just make you curious enough to dip into the early chapters to learn more about the trials and tribulations of the early pioneers of quantum chemistry. For teachers and students in a typical chemical bonding course this book should be mandatory reading – one will then get a sense of the grand scale, the key players (apart from the ones that are usually popularized), and the emotional side of what otherwise may seem as a 'dry' subject. For those who have made it a habit to indulge in making slight remarks on quantum chemistry and chemists, this book will hopefully be a sobering wake-up call. At the very least, one will gain respect for names like Erich Armand Hückel and Samuel Francis Boys. Moreover, it will bring a wry smile on the faces of instructors, even today, who attempt to present the theory of the chemical bond with some care and honesty.

SRIHARI KESHAVAMURTHY

Department of Chemistry,
Indian Institute of Technology Kanpur,
Kanpur 208 016, India
e-mail: srihari@iitk.ac.in



Plant Taxonomy: Past, Present and Future – Dr Prithipalsingh Festschrift. Rajni Gupta (ed.). Tata Energy Research Institute (TERI), TERI Press, Darbari Seth Block, IHC Complex, Lodhi Road, New Delhi 110 003. 2012. xxi + 349 pp. ISBN: 978-81-7993-359-6. Price not mentioned.

Taxonomy is truly ancient (hence known as the mother of all branches of biology!), inherently appealing for being proximal to exploring nature and invariably linked to all other branches of biology. The subject is based on certain principles and established concepts and involves both primary morphological observations and sophisticated experimentation when pursued for enquiring into allied branches for complementary support. The subject gets well synthesized and truly blooms once these are ideally and optimally fulfilled. Unfortunately, the subject has taken a retreat in majority of universities/colleges in undergraduate/postgraduate courses in the last three decades. Its teaching was neglected with curricula reformers almost denying its desired/deserved inclusion in various courses of study. This has resulted in both students and even some professors becoming unaware of both basics and identities of familiar plants. The subject survived in a few scattered universities/colleges where renowned teachers counselling for the subject are part of the faculty inspiring students to understand its grace and glory.

The subject is to be appropriately taught elucidating nuances in divergence/similarity with adequate exposure to field studies to comprehend in its integrity and perspective. Such an exposure can fairly impel students to embrace it by passion and pursue the same as a profession. The present reviewers as biologists still remember as students, running around teachers attempting to know the Latin names (Latinized names) of the collected plants, charmed by character consistency and systemized evolution in nature and in plant groups. No prospective biologist should miss this learning/experience! It is now well realized that taxonomy teaching, research and training have a bearing on documentation, monitoring and conservation of the biological resources of the country. India takes pride in the richness of these resources (as it is one of the 12 mega-biodiversity nations harbouring four of the 39 hotspots in the world) and is committed as a signatory to the Convention on Biological Diversity (CBD) to conserve it through sustainable utilization. More decentralized approaches of documentation of biodiversity resources are encouraged today to build biological inventories as quickly as possible to recognize their hitherto unknown potential uses. Member countries of CBD, known by Conference of Parties (CoP), affirmed the implementation of biodiversity strategy action plan 2010–2020 to realize 20 Aichi targets.

Capacity building in taxonomy in all the concerned areas has become a major