Preface

The Windows

In these dark rooms where I live out
empty days, I circle back and forth
trying to find the windows.
It will be a great relief when a window opens.
But the windows are not there to be found—
or at least I cannot find them. And perhaps
it is better that I don't find them.
Perhaps the light will prove another tyranny.
Who knows what new things it will expose?

Constantine P. Cavafy (1863–1933). Cavafy lived most of his life in Alexandria, Egypt, and wrote his poetry in Greek. (From: Edmund Keeley. *C.P. Cavafy.* Copyright © 1975 by Edmund Keeley and Philip Sherrard. Reprinted by permission of Princeton University Press.)

All Is Symbols and Analogies

Ah, all is symbols and analogies!
The wind on the move, the night that will freeze,
Are something other than night and a wind.
Shadows of life and of shiftings of mind.

Everything we see is something besides
The vast tide, all that unease of tides,
Is the echo of the other tide—clearly
Existing where the world there is is real

Everything we have's oblivion.
The frigid night and the wind moving on—
These are shadows of hands, whose gestures are the
Illusion which is this illusion's mother

Fernando Pessoa (1888–1935) (November 9, 1932, excerpt from notes for a dramatic poem on Faust). Pessoa lived mostly in Lisbon, Portugal, but spent part of his youth in Durban, South Africa. He wrote in Portuguese and English and used several heteronyms. (From: E.S. Schaffer, ed. *Comparative Criticism,* Volume 9, *Cultural Perceptions and Literary Values* [University of East Anglia, CUP, 1987]. Copyright © 1987 Cambridge University Press. Reprinted by permission of Cambridge University Press.)

Like many other books, this book has had a long period of gestation. We first met years ago on the other side of the Atlantic, in 1991 in Madison, Michigan, when one of us was writing the scientific biography of Fritz London and the other completing her Ph.D. thesis about the emergence of quantum chemistry in the United States. Since then, on and off, we have been discussing various aspects of quantum chemistry—of a subdiscipline that is not quite physics, not quite chemistry, and not quite applied mathematics and that was referred to as mathematical chemistry, subatomic theoretical chemistry, quantum theory of valence, molecular quantum mechanics, chemical physics, and theoretical chemistry until the community agreed on the designation of quantum chemistry, used in all probability for the first time by Arthur Erich Haas (1884–1941), professor of physics at the University of Vienna, in his book *Die Grundlagen der Quantenchemie* (1929).

Progressively, we became more and more intrigued by the emergence of a culture for doing quantum chemistry through the synthesis of the various traditions of chemistry, physics, and mathematics that were creatively meshed in different locales. We decided to look systematically at the making of this culture—of its concepts, its practices, its language, its institutions—and the people who brought about its becoming. We discuss the contributions of the physicists, chemists, and mathematicians in the emergence and establishment of quantum chemistry since the 1920s in chapters 1, 2, and 3. Chapter 4 deals with the dramatic changes brought forth to quantum chemistry by the ever more intense use of electronic computers after the Second World War, and we continue our story until the early 1970s. To decide when one stops researching, to decide what not to include is always a decision involving a dose of arbitrariness. Necessarily and naturally, a lot has been left out.

The first work that had convincingly shown that quantum mechanics could successfully deal with one of the most enigmatic problems in chemistry was published in 1927. It was a paper by Walter Heitler and Fritz London, who discussed the bonding of two hydrogen atoms into a molecule within the newly formulated quantum mechanical framework. Thus, we start our narrative *after* the advent of quantum mechanics and try to read the unevenly successful attempts to explain the nature of bonds that were made by different communities of specialists within different institutional settings and supported by different methodological and ontological choices.

The narrative about the development of quantum chemistry should not be considered only as the history of the way a particular (sub)discipline was formed and established. It is, at the same time, "part and parcel" of the development of quantum mechanics. The formation of the particular (sub)discipline does, indeed, have a *relative autonomy,* with respect to the development of quantum mechanics, but this kind of autonomy can only be properly appreciated when it is embedded within the overall framework of the development of quantum mechanics. The history of quantum mechanics is, certainly, not an array of milestones punctuated by the "successes" of the applications of quantum mechanics. Such applications should not only be considered either as extensions of the limits of validity of quantum mechanics or as "instances" contributing to its further legitimation, as in any such "application" we can think of—be it nuclear physics, quantum chemistry, superconductivity, superfluidity, to mention a few—new concepts were introduced, new approximation methods were developed, and new ontologies were proposed. The development of quantum mechanics "proper" and "its applications" are historically a unified whole where, of course, each preserves its own relative autonomy.

In a couple of years after the amazingly promising papers of Heitler, London, and Friedrich Hund, Paul Adrien Maurice Dirac made a haunting observation: that quantum mechanics provided all that was necessary to explain problems in chemistry, but at a cost. The calculations involved were so cumbersome as to negate the optimism of the pronouncement. It appears that until the extensive use of digital computers in the 1970s, the history of quantum chemistry is a history of the attempts to devise strategies of how to overcome the almost self-negating enterprise of using quantum mechanics for explaining chemical phenomena.

We tried to write this history by weaving it around six clusters of relevant issues.

During these nearly 50 years, many practitioners proceeded to introduce semiempirical approaches, others concentrated on rather strict mathematical treatments, still others emphasized the introduction of new concepts, and nearly everyone felt the need for the further legitimization of such a theoretical framework—in whose foundation lay the most successful physical theory. This composes our first cluster, one where the epistemic aspects of quantum chemistry were being slowly articulated. The second cluster is related to all the social issues involved in the development of quantum chemistry: university politics, impact of textbooks, audiences at scientific meetings, and the consolidation of alliances with practitioners of other disciplines. The contingent character in the development of quantum chemistry is the third cluster, as at various junctures during its history, many who were working in this emerging field had a multitude of alternatives at their disposal—making their choices by criteria that were not only technical but also philosophical and cultural. The progressively extensive use of computers brought about dramatic changes in quantum chemistry. "Ab initio calculations," a phrase synonymous with impossibility, became a perfectly realizable prospect. In a few years a single instrument, the electronic computer, metamorphosed the subdiscipline itself, and what brought about these changes composes our fourth cluster. The fifth cluster is about philosophy of chemistry, especially because quantum chemistry has played a rather dominant role in much of what has been written in this relatively new branch of philosophy of science. Our intention is not to discuss philosophically the host of issues raised by many scholars in the field but to raise a number of issues that could be clarified through philosophical discussions. Among these issues, perhaps the most pronounced is the role of mathematical theories in chemistry, including their descriptive or predictive character. Different styles of reasoning, different ways of dealing with constraints, and different articulations of local characteristics have been all too common in the history of quantum chemistry. These compose the sixth cluster.

Throughout the book, the references to these clusters are not always explicit, but they are certainly present in our narrative all the time. In this manner, we hope to have been able to put forth a historiographical perspective of the way one can approach the history of an in-between subdiscipline such as quantum chemistry.

We keep on reminding our students that they should never forget that any history, including history of science, is fundamentally about people. There are many such figures in the history of quantum chemistry, and we hope to have been able to bring out how the specificity of each and his or her education and role in various institutions shaped the culture of quantum chemistry. The complex processes of negotiations concerning all sorts of technical and conceptual issues that molded the flexible and at times elusive identity of quantum chemistry may be traced in the multifarious activities of these people.

One of the truly difficult parts of writing about the history of the physical sciences is the extent of the technical details to be included. It is one of those "standard" problems, which, nevertheless, needs to be clarified and specified every time. The problem becomes even more difficult when the interpretation of the technical parts of the works involved in such a history does not have any "grand" implications and, hence, cannot be intelligibly put into plain language. Time dilation, length contraction, the curvature of space, the discreteness of atomic orbits, the uncertainty principle, and the reduction of the wave packet are exceedingly complex notions that, nevertheless, can be reasonably well described and discussed without, in a first approximation, having to resort to the mathematical details behind them. It is obviously the case that we do not imply that whoever decides to write about these subjects without the heavy use of mathematics is guaranteed to do a good job. Quite the opposite is the case, and the misunderstandings and myths around these subjects are mostly due to such popular writings. Popularization does require the effective use of language—but it also requires much more. Nevertheless, there have been excellent popular accounts of these developments, and what is more important, there have been superb scholarly works where use of the technical background was optimal for comprehension of the implications of the theory. How, though, does one go about to explain the work of scientists whose extremely significant contributions are inextricably tied up with the understanding of the technical details? If one knows nothing about the subject and does not have any training in the general area of the subject matter, then it is impossible to learn the subject by just reading the history of the area, no matter how conscientiously the authors present the technical details. In contrast, for those readers who either know the subject or can follow the technical details because of their training, what is included may appear to be a rather watered down version that does not do much justice to the wealth of a particular formulation. There is, obviously, no standard rule or prescription of how to get out of this Sisyphean deadlock. The decisions we took as to how to present the technical details depended on what we believed to be pertinent every time such a problem arose while keeping in mind that whoever will be interested in reading the book should be able to read it without having to follow closely the technical details.

By the time of the 1970 Conference on Computational Support for Theoretical Chemistry, which discussed how computational support for theoretical chemistry could be efficiently achieved, it was clear to all quantum chemists that a long way had been traversed since the publication of the Heitler and London paper in 1927. The “theory of resonance” proposed by Linus Pauling and the molecular orbital approach developed by Hund and Robert Sanderson Mulliken had been systematically elaborated, a host of new concepts had come into being, and many and powerful approximation methods were being extensively used in a complementary manner. Many quantum chemists started dealing with large and complicated molecules. Chemistry, it appeared, might not have acquired its “own” theory by the physicists’ standards, but certainly, quantum mechanics did provide the indispensable framework for dealing with chemical problems. Dirac, after all, might have turned out to be right.

The computer had forced many practitioners to rethink the status of theory vis-à-vis inputs from empirical data and more or less approximate calculations, and visual imagery acquired a new physical support and heralded new applications. Experiments took on new meanings: Many ab initio calculations “substituted” for experiments, and mathematical laboratories became part of the new sites of quantum chemistry. Institutionally, the discipline became truly international, and its new cohesive strength arose from a successful networking crossing continents, generations, practitioners’ research areas, and different and at times antagonistic modes of reasoning. In a very short time, the possibilities provided by the new instrument brought about a realization that the future of the subdiscipline would be radically different than its past: Gone were the days of discussions and disputes about conceptual issues and approximation methods, and the promised future was full of numbers expressing certainties rather than signifying semiempirical approaches.

Our historical and historiographical considerations have been shaped through a “dynamic conversation” with a number of historical works. John Servos’s *Physical Chemistry from Ostwald to Pauling* (1990), Mary Jo Nye’s *From Chemical Philosophy to Theoretical Chemistry* (1993), and aspects in Thomas Hager’s biographical studies (1995, 1998) on Linus Pauling represent some of the first works where historical issues of quantum chemistry began to be discussed. A number of Ph.D. dissertations have dealt with facets of the history of quantum chemistry: Robert Paradowski (1972) offered a comprehensive analysis of Pauling’s structural chemistry; Buhm Soon Park (1999a) concentrated on the study of the role of computations and of computers in reshaping quantum chemistry; Andreas Karachalios (2003, 2010) offered a detailed study of Erich Hückel; Martha Harris (2007) argued that the chemical bond, as explained quantum mechanically, became a signifier of disciplinary change by the 1930s, distinguishing the new quantum chemistry from the older physical chemistry; and Jeremiah James (2008) has discussed Pauling's research program at the California Institute of Technology during the 1920s and 1930s.

Scholars, including many colleagues and various chemists, who wrote papers, chapters in books, dictionary entries, recollections, biographical memoirs, autobiographies, obituary notices, or gave interviews have provided us with a wealth of information often following different methodologies. Furthermore, there are a number of works where some historiographical issues have been tackled. The discussion of the emergence and development of quantum chemistry in different national contexts has been given considerable attention. Studies offering comparative assessments of some protagonists' views and practices include analyses of Pauling and George W. Wheland's views on the theory of resonance; of the different contexts of the simultaneous discovery of hybridization by Pauling and John Clarke Slater; of the contrasting teaching strategies of Charles Alfred Coulson and Michael J. Dewar; as well as of Pauling and Coulson as seen through their famous textbooks *The Nature of the Chemical Bond* and *Valence*, respectively. The period after the Second World War has not yet been systematically studied, except for preliminary assessments of the impact of computers in the methodological, institutional, and organizational reshaping of quantum chemistry. Furthermore, quantum chemistry has provided ample material for much of the discussion in the philosophy of chemistry, and various problems pertinent to philosophy of chemistry, most prominently that of reductionism, have been addressed from a historical perspective.

Over the years, a number of scholars have worked on topics related to the history of quantum chemistry. Their work and the conversations with some have been an inspiration and an immense help for us. We especially acknowledge the work of Steven G. Brush, who introduced one of us to the history of quantum chemistry, on Hückel and benzene; of Andreas Karachalios on Hückel and Hellmann; of Helge Kragh on Bohr, Hund, and Hückel; of Mary Jo Nye on the history of theoretical chemistry; of Buhm Soon Park on the different genealogies of computations; of Sam Schweber on Slater; and of J. van Brakel, Robin Findlay Hendry, Jeff Ramsey, Eric Scerri, Joachim Schummer, and Andrea Woody on the philosophical considerations of issues in quantum chemistry. While writing the book we received many comments and much advice and support from many colleagues and friends. We thank Jürgen Renn for his hospitality at the Max Planck Institute for the History of Science (MPIWG) and for the use of the services of its excellent library. Robert Fox and José Ramon Bertomeu Sanchez have contributed in different ways to hasten us in the period that gave way to the last stage of this long journey. Theodore Arabatzis read the manuscript and offered valuable comments. Jed Z. Buchwald was particularly supportive of our project from the very beginning and accepted our proposal to include the book in the series he directs. Patrick Charbonneau made a number of incisive comments. Referees made perceptive comments and very useful suggestions. We thank them all.

Along this journey, various chemists and scientists have contacted us, offering their memories and comments. We thank them all, and especially J. Friedel, who commented on the sections about French quantum chemists. The oral interviews assembled on the Web page created by Udo Anders have been very helpful, as well as Anders Fröman's and Jan Lindenberg's recollections. The last year of research depended on the constant support of Urs Schoeflin, the librarian of the MPIWG, and his staff, as well as on Lindy Divarci, who took care of our requests; on the librarian Halima Naimova from the Astronomical Observatory of Lisbon; on Michael Miller, technical archivist at the American Philosophical Society; and on Daniel Barbiero, manager of archives and records at the National Academy of Sciences. We thank them all.

Our professional lives in Greece and Portugal are interlaced with all kinds of activities for the further entrenchment of our discipline, and, thus, often we had to stop the project to get involved with time-consuming yet necessary undertakings in the precarious institutional environment for such subjects as history of science and technology. But in all these instances, we have been privileged to be surrounded by colleagues who are truly excellent scholars with whom we share the same views as to the ways our discipline will continue to be strengthened within our local conditions and with whom we have good friendships. We specifically thank Ana Carneiro, Luís Miguel Carolino, Maria Paula Diogo, Henrique Leitão, Marta C. Lourenço, Tiago Saraiva, Theodore Arabatzis, Jean Christianidis, Manolis Patiniotis, Faidra Papanelopoulou, and Telis Tympas. We have also been involved in many projects that did not intersect with quantum chemistry. Perhaps the most satisfying and enjoyable was the creation and a fruitful first decade of the activities of the international group Science and Technology in the European Periphery (STEP).

We thank the families of Fritz London and Charles Alfred Coulson, who have kindly provided us with photographs, and Mariana Silva for preparing the diagrams for publication. We also thank Professor W. H. E. Schwarz for his help. At long last, writing a joint book, kilometers apart, in two extremities of Europe emerged from the world of dreams into the real world. We hope our readers will find this book useful. We enjoyed each and every step of the convoluted process leading to it, from e-mail discussions to phone conversations to a very long discussion ironing out all the difficult problems related to the book at "another" in-between site—a cafe situated between Hagia Sophia and the Blue Mosque in Istanbul.

The shaping of scientific disciplines is mediated by people, their choices, allegiances, and conflicts, as well as by their changing networks of interactions. But certainly, identity search and identity crises are neither primarily nor exclusively associated with them. During a dinner in Lisbon with our partners Eleni Stambogli and Paulo Crawford, we talked about the movie *When Cavafy Met Pessoa* (directed by Stelios Charalambopoulos), which is about the amazingly similar lives of these two contemporaneous poets, exquisite explorers of the human nature, so prized in Greece and Portugal and who had never met. The choices that led to the poems at the beginning of the book are, perhaps, the only thing that each author has done independently. Otherwise, what is in the book has been untirelessly discussed and reflects the views of both.

Some of what has already appeared in a few of our published works has been expanded and reworked in this book. In chapters 1 and 2, we drew from our papers "The Americans, the Germans and the Beginnings of Quantum Chemistry: The Confluence of Diverging Traditions" (*Historical Studies in the Physical Sciences* 1994;25:47–110); "One Face or Many? The Role of Textbooks in Building The New Discipline of Quantum Chemistry" (in Anders Lundgren, Bernadette Bensaude-Vincent, eds. *Communicating Chemistry. Textbooks and their Audiences, 1789–1939*, Science History Publications, 2000, pp. 415–449); and "In Between Words: G.N. Lewis, the Shared Pair Bond and Its Multifarious Contexts" (*Journal of Computational Quantum Chemistry* 2007;28:62–72).

In chapter 3, we drew from our papers "Quantum Chemistry *qua* Applied Mathematics. The Contributions of Charles Alfred Coulson 1910–1974" (*Historical Studies in the Physical Sciences* 1999;29:363–406); and "Quantum Chemistry in Great Britain: Developing a Mathematical Framework for Quantum Chemistry" (*Studies in the History and Philosophy of Modern Physics* 2000;31:511–548).