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BOOK SYMPOSIUM

Historical and philosophical perspectives on quantum chemistry

Kostas Gavroglu and Ana Simões: Neither physics nor chemistry: A history of quantum chemistry. Cambridge, MA: The MIT Press, 2012, xiv+351pp, $40.00, £27.95 HB

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In this book, Gavroglu and Simões offer a definitive account of the history of quantum chemistry, the like of which is not to be found anywhere in the extant literature to the best of my knowledge. It is a pleasing and impressive culmination of 20 years of work, a new synthesis which develops and brings together numerous previous publications by the authors into a coherent and comprehensive whole. It is based on extensive and painstaking studies of both secondary and primary sources (published and archival), as the well-balanced 48-page bibliography easily attests. Various fascinating strands of development are recounted and reconstructed, with meticulous technical detail and also with instructive attention to the biographical,

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institutional, and sociopolitical factors that shaped the technical developments. The authors stress the contingency in the scientific developments they discuss and do not force a deterministic historiography on the material. For example, it is surely instructive to learn that much support for quantum chemistry came from the US military research-funding agencies, while Charles Coulson, one of the most influential leaders in the field internationally, was a deeply religious pacifist; there is no clear-cut way of tidying up such stories, and the authors are correct in not doing away with the untidiness.

The main purpose of this review is to serve as a user's guide to potential readers so that they can get the most out of this book. I freely admit that I have little expertise in quantum chemistry and its history; however, I think the blind can sometimes lead the blind effectively, and precisely thanks to blindness. In that spirit, this review contains some suggestions to novices in quantum chemistry and its history, from a fellow novice, as to how to make the best of this enormously rich work that will seem quite formidable and difficult to get into if one lacks a previous background in the subject. The novices I have in mind include those who know quite a bit of modern physics but not chemistry, and those who know something about pre-quantum chemistry, but not much about modern chemistry. Such categories of readers may not think that the history of quantum chemistry is something they ought to study, but I think they would benefit greatly from studying this book seriously.

Quantum chemistry is an intricate subject; so is its history. Accepting the difficulty and complexity is the first productive step for the novice in tackling this book. Do not expect to be able to read it quickly or casually, and do not expect the narratives to have simple structures or tidy endpoints. The main chapters (1–4) are very long and technical narratives which may be best read with clear overall directions already in mind. The brief introductory chapter helpfully pulls out some of the main themes covered in the rest of the book, but they may not mean all that much to the novice who has not yet digested the main chapters; it may be helpful to read the final chapter first, where the authors reflect on some of the most important historical and philosophical trends concisely, but more concretely than in the Introduction.

Not all technical details need to be followed closely to get the gist of what the authors are trying to convey. And some technical things are actually not as hard as they seem, and the novice reader will be greatly helped by the simple discipline of taking the trouble to look up some technical concepts that can be briefly explained at an intuitive level—this is easy enough to do especially in this age of the internet. So, for example, there is no need to be daunted by unexplained terms like homopolar bond, fractional bond order, and π and σ orbitals—just look them up, though I wish the authors would have provided a glossary. Some concepts (e.g., resonance) are truly difficult, and in such cases, the authors guide us expertly and patiently through the ins and outs of the concepts and the debates surrounding them. The tracing of developments in such cases constitutes some of the most valuable and exciting contributions of this book.

Contrary to the appearance that may be given by a casual glance through the main chapters, this is a deeply philosophical book. I think a serious study of it will yield handsome dividends to the philosophical reader—not only interesting examples against which to pit various standard debates in the philosophy of science, but also a fresh stimulus for new ideas and questions. Historians and philosophers of science have tended to neglect quantum chemistry and other "in-between" disciplines (261). But modern science is full of such disciplines, and learning more about them will be a good antidote to the exaggerations and distortions in our philosophical picture of science that come from having thought too much about simpler cases like Newtonian mechanics and special relativity. If we allow ourselves to be educated through a serious study of this book, we will think better and very differently about venerable old philosophical issues such as reductionism, realism, pluralism, operationalism, pragmatism, and the role of mathematics in science. I would like to summarize and highlight Gavroglu and Simões's discussion of some of these issues here, since they are developed in a slow and somewhat scattered way through the intricate narratives in the book.

As the main title of the book indicates, the relation between chemistry and physics is a foremost theme for Gavroglu and Simões. First of all this is a question of reductionism: Is chemistry just applied physics, and did that reductionist dream become a reality with the advent of the electron, and even more with the coming of full-fledged quantum mechanics in the late 1920s? Much scientific and philosophical thinking has been haunted by the reductionism that was so memorably voiced by Paul Dirac in 1929: "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." (9) Gavroglu and Simões caution against using this sort of reductionism as a guide for our historiographical and philosophical thinking, adding to the voices of some other prominent philosophers and historians such as Eric Scerri, Mary Jo Nye, and Theodore Arabatzis[1]. And they do so not by explicit philosophical arguments of their own, but by displaying the elaborate struggle with reductionism on the part of some of the towering figures in quantum chemistry.

It is very instructive to learn that Linus Pauling's great success in shaping the early directions of work in this field was due to his ability to *use* quantum-mechanical ideas to help him do better *chemistry*, rather than turning chemistry into applied physics. Strikingly, Pauling thought of his resonance theory as a direct continuation of nineteenth century organic structural chemistry, dubbing it "modern structural chemistry" (77). He declared in a retrospective in 1970: "The theory as developed between 1852 and 1916 retains its validity…. It has been developed almost entirely by induction (with, in recent years, some help from the ideas of quantum mechanics developed by the physicists). It is not going to be overthrown" (251). And Gavroglu and Simões tell us that Pauling's emphasis on the tradition of structural theory was due to its continuing importance in organic chemistry, and its newfound usefulness in the applications of chemistry in biology and medicine—one is reminded of his great success in elucidating the alpha-helix structure of proteins and his role in the race to solve the problem of DNA structure. In the "integration"

[1] See, for example, Scerri (2008, Section A), Nye (1992), Arabatzis (2006, Chapter 7).

of the sciences that he advocated, to be achieved through the sharing of tools and methods, Pauling saw chemistry, not physics, as occupying the central place (119). Pauling's anti-reductionism concerning the chemistry–physics relation was shared by Charles Alfred Coulson, the clear leader of the field in Britain, who said in 1970 that "one of the primary tasks of the chemists during the initial stages in the development of quantum chemistry was to escape from the thought forms of the physicists" (1). Generally speaking, while most twentieth century chemists accepted that the momentous developments in physics had some serious implications for the practice of chemistry, there were a variety of ways in which that relevance of physics to chemistry was understood and developed.

Complicating the story of reductionism in this way also allows Gavroglu and Simões to pay proper attention to the pluralism present within quantum chemistry. In this regard, Coulson emerges as the most intriguing figure—a veritable philosopher as well as a consummate applied mathematician and builder of scientific communities. Gavroglu and Simões describe him as "a stubborn and committed advocate of methodological pluralism, of the possibilities for exploring different approaches in different problems, always eager to compare and contrast them" (226–227). Coulson even had a striking chemical metaphor for the benefits of pluralism (reminiscent of C. S. Peirce's metaphor of cables): "the validity of the scientist's account depends on the degree of interlocking between its elements", just as "the strength of an artificial fiber depends on the degree of cross-linking between the different chains of individual atoms" (259). Various other leaders in the field, including John Slater and John Hasbrouck Van Vleck, also shared such pluralism, recognizing both the valence bond (VB) approach and the molecular orbital (MO) approaches as different approximations, each of them valid and useful (92–97). The competition between VB (developed by Pauling building on the ideas of Gilbert Newton Lewis) and MO (pioneered by Robert S. Mulliken) is a central theme in the story of quantum chemistry, and readers who are not familiar with these theoretical approaches should try to read up on the basics: Even 10 minutes spent on the internet will make a big difference in following the discussions in this book. As it turns out, the relationship between VB and MO was a very difficult question that the quantum chemists themselves grappled with for a long time without a clear resolution or consensus. With lasting uncertainty on such a fundamental point, it is not a surprise that many quantum chemists retained at least a degree of pluralism. Per-Olov Lödwin in Sweden had a clear and energetic vision for the future of quantum chemistry, but also emphasized that "various types of theories are constructed for different purposes" (219). In France, Alberte and Bernard Pullman and their collaborators also sounded a clear note of methodological pluralism: "We hope to have made clear that any method should be used with caution and that hasty critical statements should be avoided" (197). And the pluralism that our authors see in the thinking of some of their historical heroes links up interestingly with their own historiographical pluralism, which they take as "a truly liberating lesson" (7).

Along with pluralism came a loosening of realism. Dirac's reductionist vision, which had excited the thinking of the initial pioneers of quantum chemistry including Walter Heitler, Fritz London and Friedrich Hund, was based on a firm realist commitment to the truth of fundamental physics. But despite the lip service that many chemists continue to pay to the idea of fundamental physics as the ultimate basis of chemistry, faith in the ultimate truth of physics turned out not to be of much use to those who wanted to find more effective ways of answering chemical questions. As chemists found their own ways of working, they also became less restrained in choosing what they believed to be real. Actually I think quantum mechanics itself helped in this regard, by shaking up the fundamental concepts of physics in such a serious way. For example, as Mulliken rightly pointed out, quantum mechanics suggests that only the whole molecule (if that) should be regarded as real, not the atoms or ions that allegedly make up the molecule (85). If even *atoms* are only useful conceptual abstractions rather than simple realities, why should the chemists feel obliged to regard anything else as unchallengeably real? As one can expect, interesting and subtle debates ensued. For example, Pauling and his close collaborator George W. Wheland had a deep disagreement on this issue. Wheland argued that resonance was a “man-made concept”, not “a real phenomenon with real physical significance”; he opined that “even the double bond in ethylene seems to me less ‘man-made’ than the resonance in benzene” (124). Pauling countered that all these concepts were equally man-made, and there was no reason to disparage the resonance concept particularly. Coulson jumped in with his view that resonance was “quite definitely” not a real phenomenon, “merely a way of dissecting” the solution of the relevant Schrödinger equation (166). Coulson seems to have been troubled by an operationalist conscience, as his Oxford inaugural lecture from 1952 shows: “remember, no one can ever measure the spin of a particular electron [inside an atom]!”—“remember, there is no way of distinguishing experimentally the density distribution of one electron from another!”—a bond is “no more real that the square root of –1!” A few years later he wrote with enduring anti-realist caution: “Sometimes it seems to me that a bond between two atoms has become so real, so tangible, so friendly that I can almost see it. And then I awake with a little shock: for a chemical bond is not a real thing: it does not exist: no-one has ever seen it, no-one ever can. It is a figment of our own imagination” (181–182).

It would be unproductive to become mired in the realism debate too deeply here, and the quantum chemists themselves did not, for the most part. Gavroglu and Simões point out that what came to be “almost universally accepted by the chemical audiences” was a “(semi)phenomenological approach” originating from America (encompassing both BV and MO), with an “intense pragmatic streak” (39). But pragmatism did not mean a lack of theory or philosophical reflection. Many leading quantum chemists engaged in serious and innovative ways in the business of concept-building. Coulson is illuminating here, again. He saw his line of work as applied mathematics, the “nature” of which was to discover the “inner structure and form” of the physical world. He regarded “the real function of applied mathematics” as “the formulation of the concept”, and its progress as consisting in imagining “a new set of concepts to transcend the old” (175–176). It is a common error to see only a technician’s job in applied mathematics, especially the numerical side of the business. (Or rather, perhaps we should stop denigrating what technicians do.) I must admit that there was something of this error in my own head when I started reading this book, as I was surprised at how philosophical the content of Chapter 3 was—it is titled "Quantum Chemistry *qua* Applied Mathematics: Approximation Methods and Crunching Numbers". The history of quantum chemistry could be seen as a long struggle to work out various mathematical methods; this is a pragmatic sort of business at one level; but at another level, what really matters is physical interpretation, and this is creative work aimed at understanding. John Edward Lennard–Jones exhorted his audience at the 1954 meeting of the British Association for the Advancement of Science not to forget the chemistry buried in the tangle of mathematics in theoretical chemistry: "the task remains clear and insistent … to express as simply and clearly as possible the physical meaning of the mathematical theories that have swept through the whole of chemistry" (153).

In highlighting several themes above, I have neglected much in the rich tapestry of the book, which was only in the interest of pulling out some of the threads that I think may be missed by many readers otherwise. To get the full benefits of the book, there is of course no other way than reading it in detail. I believe this book will be the standard work on the history of quantum chemistry for many years to come, both an incredible resource and a clear benchmark for current and future research. It should be a deeply rewarding read for a wide variety of scholars and students.

Jeremiah James

Let's not mince words: *Neither Physics nor Chemistry* is a disciplinary history. This might seem a bit strange given the present climate in the history of science and science studies. "The end of disciplines" is a fashionable topic in some circles (see de Chadarevian and Rheinberger 2009; Chandler and Davidson 2009), and likewise, many of the terms we now use when discussing late twentieth century science undermine traditional notions of disciplines and their role in the sciences. Think, for example, of the implications for disciplines, native as they are to academe, of terms such as "technoscience" or "mode two research" (Latour 1987; Gibbons et al. 1994). Properly applied, however, these terms and their attendant critiques do not demand the expurgation of disciplines from the history of science tout court. Rather, they aid us in developing historical perspectives on the emergence (and possible end) of disciplines, defining for them a proper era, place, and role[2]. And in the years 1927–1970, the elite research universities of Europe and America upon which Kostas Gavroglu and Ana Simões focus their study not only hosted an array of scientific disciplines with roots deep in the nineteenth century but also welcomed newcomers such as molecular biology, solid-state physics, and quantum chemistry. The "end of disciplines" only makes questions related to why and how these disciplines emerged all the more pointed, and these are chief among the questions Gavroglu and Simões address in their history of quantum chemistry. Its publication is quite timely.

[2] Some scholars do attempt to extend these critiques almost indefinitely into the past. Although boundary transgressions have clearly always been part and parcel of the disciplinary system, one can still meaningfully distinguish between these earlier transgressions and threats to the disciplinary system as a whole.

Of course upstarts like molecular biology or radio astronomy were in important ways dissimilar from the classical disciplines of the second scientific revolution and from the host of (sub)disciplines formed around the turn of the century. For Gavroglu and Simões, quantum chemistry was similarly dissimilar, and that is one of the keys to understanding its development. They present quantum chemistry as a quintessential "in-between" discipline, with evolving ties to chemistry, physics, and applied mathematics, and hence with its disciplinary filiation and affiliations often at odds, unclear, or in dispute. Moreover, they make appraisal of these peculiarities the rubric for their account. Their emphasis is on the "in-between." This leads to a tale that will appear in some respects familiar to those acquainted with other disciplines that emerged in the early to mid-twentieth century. While other details of the account discourage too hasty generalization about this, arguably last, generation of scientific disciplines. In the absence of a general theory or model of the decline and demise of the disciplinary framework (potential or actual), balanced histories like the one Gavroglu and Simões provide offer perhaps the best means to building up our understanding of the historical contingency of this mode of organizing knowledge and knowledge production.

To be fair, this does not appear to be the authors' prime motivation. They are somewhat circumspect about the potential for generalizing their approach to other in-between disciplines (7). Their interests clearly lie more in chronicling the specific development of quantum chemistry and evaluating its relevance for chemistry and neighboring disciplines than in a general investigation of disciplines or "disciplinarity". *Neither Physics nor Chemistry* presents not a case study in the emergence of scientific disciplines, but a meso-history focused on an object larger than a local culture (e.g., a laboratory) and yet smaller than the always nebulous (if not illusory) "scientific community". Moreover, as with true microhistories, this approach has the potential to show us, as Lorraine Daston put it, "the universe in a grain of sand" (Daston 2009, 809), by articulating insights that take shape, not because of dedication to one or another "grand generalization", but through intimate contact with the details of the instance at hand.

Gavroglu and Simões make no mystery of the views they developed through their encounter with quantum chemistry and the manner in which these structure their narrative. They dedicate their introduction to presenting six "clusters of issues" that they view as the binding threads of the narrative that follows: "the epistemic content of quantum chemistry, the social issues involved in disciplinary emergence, the contingent character of its various developments, the dramatic changes brought about by the digital computer, the philosophical issues related to the work of almost all the protagonists, and the importance of styles of reasoning in assessing different approaches to quantum chemistry" (7). Given its central role in the final chapter on historiographical considerations, "the role of theory in chemistry" probably deserves a place on the list as well, but it is not an obfuscatory omission. It is clearly an eclectic list, and the authors are careful to point out that its members are not distributed or treated equally throughout the book. The role of computers is restricted almost completely to the fourth chapter and the historiographical conclusion, and the discussion of social factors is, to a somewhat unfortunate degree, concentrated in these same places. The eclecticism of the list, however, does not unmoor the authors' account. On the contrary, it evinces a strong commitment to a polyvalent, distinctly historical notion of disciplines, clearly informed by the insights historians of science developed during the 1990s (e.g., Nye 1993a, b; Lenoir 1997), after they had turned away from the borderline monocausal models of the mid-twentieth century (Lemaine et al. 1976) and recovered somewhat from the initial shock and glamour of their encounters with the likes of Pierre Bourdieu and Michel Foucault.

Unlike most of its twentieth century antecedents, however, *Neither Physics nor Chemistry* can forgo the lengthy explanation and defense of the (now much less controversial) multifactorial outlook. Gavroglu and Simões present instead a narrative that aims to instantiate this outlook, not only in its individual episodes and analyses but also in its overall narrative structure. In keeping with their emphasis on the in-between nature of quantum chemistry and the *fin-de-siècle* realization that disciplines are rarely, if ever, the product of single individuals, institutes, or discoveries (Lenoir 1997), the first three chapters—titled quantum chemistry *qua* physics, chemistry and applied mathematics, respectively—present overlapping, semi-sequential tales of the relatively autonomous research communities that only in conglomerate constituted prewar quantum chemistry. It is a refreshing and innovative format for a disciplinary history.

The chapter titles undersell somewhat the complexity of the communities upon which they focus and the divisions between them. The authors highlight not only differences in disciplinary affiliation and career trajectory between the protagonists of the various chapters but also differences in their "styles of reasoning". Overall, I find the authors' use of this term ambiguous—styles of reasoning vary in size throughout the book to cover everything from individual theories to entire disciplines and beyond. Here, however, the term is used constructively to refer to differences between local communities in research standards and values of the sort whose importance has been showcased in the work of Peter Galison, among others (Galison 2004). The chapter divisions also embody an implicit but deep commitment to the importance of national boundaries. The three chapters could just as easily have been labeled quantum chemistry in the German(-speaking), American, and British contexts. This should not be mistaken for a return to the "national styles" of old. Gavroglu and Simões ground their portrayal of national differences in the peculiarities of small networks of local cultures that grew up around a few key research centers in each nation, not in caricatural national stereotypes (cf. Nye 1993a, b). These small networks may appear too large for true microhistory and are certainly too small for traditional uses of statistics and sociology, but in the hands of the authors, they are objects of just the right scale to track the interactions that fueled the growth of distributed research communities with partially shared values and practices—communities that in turn formed a precondition for the transformation of quantum chemistry from a research "topic" or "field" into a stable, fully fledged discipline.

Within each of their three subject research communities, Gavroglu and Simões focus on key publications and technical developments, as well as the philosophical questions and intergroup tensions these not infrequently elicited. Moreover, the authors have chosen to focus on developments that highlight the contemporary epistemic concerns of the incipient discipline and the differences in style between the different communities. Readers looking instead for a “complete” survey of developments in quantum chemistry will likely be disappointed by the absence or cursory treatment of topics such as the Born–Oppenheimer approximation, which would become the butt of several pointed methodological critiques in the years *after* the close of the authors’ tale (Sukumar 2009). But such omissions help the authors to maintain their focus on the development of quantum chemistry as an in-between discipline and on the origins of its iconic status for discussions of the role of theory and of reductionism in chemistry. However, the limited attention given institutional and extra-scientific social factors in these early chapters is troubling at points. For example, the authors do not offer a general analysis of the effects of National Socialist policies on the nascent German quantum chemistry community, despite the fact that three of the main protagonists of their first chapter (Walter Heitler, Hans Hellmann, and Fritz London) all departed Germany in response to the first round of anti-Semitic legislation promulgated in 1933, as did several more senior researchers who had offered support to the new field, such as the physicist Max Born.

Gavroglu and Simões change style considerably for their final historical chapter, “Quantum Chemistry *qua* Programming”, where they draw together the three strands of their earlier narrative and formulate their general stance on the formation and stability of in-between disciplines. This chapter is much richer in detail on the institutional siting and support for quantum chemistry. And though the chapter focuses on the transformation of quantum chemistry into a more stable, less fractious, international research community, the authors still manage to foreground the distinguishing characteristics of each contributing national element and, to a lesser extent, those of each individual research center. The objects and events that mark this transformation Gavroglu and Simões treat in ample detail. Most are commonplace for fields and disciplines that blossomed in the early postwar years: sponsored conferences at locations such as Shelter Island and the NIH, standing summer schools for research methods, textbooks suitable for students of various levels—all pitched at an international market. These were remarkably effective at overcoming the earlier tensions between the separate cultures of quantum chemistry and fusing them into a discipline. But the authors present this success as primarily the result of a generational change and of the technical success and methodological uniformity engendered by the advent of large-scale computing. It is an explanation more than a little reminiscent of Kuhn’s explanation of paradigm adoption (Kuhn 1962), and though certainly part of the story, alone it does not appear adequate to explain the peculiar success of quantum chemistry in establishing and maintaining a distinct disciplinary identity at a time when disciplines on the whole were arguably losing ground as a system for organizing scientific research.

That omission notwithstanding, the chapter contains a wealth of insights into postwar quantum chemistry, some of which highlight its peculiar character as an in-between discipline, while others shed new light on general postwar trends in the development of the physical sciences in the USA and Europe. Moreover, the authors manage, *pace* their own apprehension (x–xi), to present these at a level of technical detail that should make it accessible to most historians of modern science, but that still allows them to characterize the culture of quantum chemistry precisely enough to lay the groundwork for meaningful comparative analyses. On the one hand, Gavroglu and Simões present a constellation of conferences, textbooks, and the transformative potential of large-scale computing familiar from late twentieth century physics. On the other hand, the authors highlight the ways in which quantum chemistry clearly was not, to parody Clausewitz, "physics pursued by other means" (or to other ends). The most obvious of these were the explicit efforts of leaders in the field to escape from the "thought forms of the physicist", as Charles Coulson put it (261), and the role these efforts played in the technical success of the discipline. But no less distinguishing were factors like the prominence of Alberte Pullman (née Bucher), central figure in the founding of one of France's two leading quantum chemistry groups, and the struggle quantum chemists faced to secure "big science" funding and computing time in the shadow of nuclear physics and other cold war mainstays. These serve as clear reminders of the dangers of overgeneralization even within a range as restricted as the physical–mathematical sciences of the postwar era.

The final chapter also treats the reader to the "happy ending of a tortuous journey" (245), a resolution of the intercommunal tensions and the recurring doubts engendered by mathematical complexity that characterize the first three chapters. But the normative aspect of the preceding quote points to one problematic aspect of Gavroglu and Simões's account. In certain key respects, the authors hew too closely to the viewpoint of later practitioners of the discipline. This is particularly visible in their selection and categorization of specific works as "quantum chemistry". In the earlier chapters, they occasionally present publications in a manner that implies their justification through communities or even disciplines yet to be formed. As history is written for and from the present, there is no fault in selecting actors and articles based on their later appropriation by a given discipline, but in many cases, contributing to "quantum chemistry" clearly was not (and could not have been) the goal of the actors themselves. Given the care with which they distinguish the professional origins of their protagonists, it is somewhat surprising that Gavroglu and Simões gloss over the explanations for the significance of their research that these scientists provided before quantum chemistry, as such, could have been a motivating factor. Why did even a small group of German theoretical physicists in the late 1920s see physical explanations of valence forces (or van der Waals forces, or molecular structure) as worthy of their attention? What motivated reviewers and editors to support and publish these articles? Without answers to questions like these, it is difficult to grasp what the authors mean when they write of "the failures of the different (sub)cultures (physics and applied mathematics) to appropriate [quantum chemistry]" (246), and the cogency of their argument for the contingency of the present form of quantum chemistry suffers.

Gavroglu and Simões handle their relationship to actors' viewpoints more adeptly in their discussions of philosophical issues. They conscientiously inform the reader that they have no intention of presenting an "objective" evaluation of the philosophical problems at stake in the development of quantum chemistry, but aim instead to understand their development historically (247). Brief asides on issues relating to philosophy of chemistry occur throughout the historical sections, carefully placed in the context of the scientists who encountered and debated them. However, the real locus of Gavroglu and Simões's philosophical analysis is their concluding chapter, which focuses chiefly on the meaning and role of theory in chemistry. The chapter could almost stand alone as a position paper on the topic. A two sentence summary of the authors' viewpoints could only present an unfair caricature. Instead, suffice it to say that they raise pointed questions concerning whether key aspects of our understanding of theory, for example, its relationship to experiment or its reliance upon certain forms of reductionism are not ill-fitted to the role of theory in chemistry. It is a strong, possibly provocative stance, and in light of the central role of theory in quantum chemistry and of quantum chemistry in chemical theory, it provides new significance to the tale they tell in the preceding chapters.

It is, nevertheless, somewhat queer that this philosophical position, however worthy, overshadows the general observations the authors hazard concerning disciplines or even in-between disciplines in their concluding chapter. The structure of the book as a whole, as well as the content of its individual chapters, suggests that the emergence of new research fields and disciplines, viewed through the proper lens, may offer a new way for us to interleave and thereby "scale up" our microhistories, without resorting to outmoded top-down views or pat generalizations. Gavroglu and Simões present an example of one strategy for reinterpreting "context" as a product of relationships between local cultures rather than a semi-autonomous, comparatively static medium within which these cultures are embedded. Moreover, the specific subject the authors have chosen offers the opportunity to develop even greater *historical* insight into the "integration" of local scientific cultures, as it appears to sit at the cusp of a major change in how scientists and their supporters defined and achieved this integration. But their terse explanation of the convergence of quantum chemistry communities and their reticence regarding disciplines in the conclusion leaves some doubts concerning how and why quantum chemistry developed the kind of unity and autonomy definitive of disciplines, rather than, for example, remaining a perennial interdisciplinary field like materials science. This appears something of a missed opportunity, but it by no means detracts from the carefully researched and ingeniously structured history that Gavroglu and Simões present.

Paul Needham

Gavroglu and Simões's book traces the history of the development of quantum chemistry as it developed from Heitler and London's 1927 paper on the hydrogen molecule, which pointed toward a foundation in quantum mechanics of Gilbert Lewis's covalent, electron-pair bonding, up to the state of the art around 1970. The fundamental problem for the would-be quantum chemists was that the application of quantum mechanics required the solution of the appropriate Schrödinger equation. But a proper analytic solution could only be given for the simple case of the isolated hydrogen atom[3]. In order to address the classical issues of chemical combination,

[3] Gavroglu and Simões (3, 257) say that an analytic solution has also been given for the Helium atom. But as I understand the matter, this is a many-body problem which doesn't have an analytic solution. The authors seem to confirm this when they say "Slater … tried to carry out more accurate calculations than those of Heisenberg for the helium atom … [and later] Hylleraas … developed a more accurate method to treat the helium atom" (88).

approximation methods were needed. This called for more than strictly numerical integration, and the methods that were developed relied on additional assumptions, over and above the strictly quantum mechanical principles. Thus, Heitler and London began with the "clamped nucleus" assumption that the two electrons moved around two nuclei which were essentially fixed in space and whose positions therefore could be dropped from the calculation, and made the further assumption that the electronic wave functions could be approximated in terms of products of atomic electronic wave functions of which linear combinations could be taken. The half-integral spin of the electrons meant they were subject to the Pauli exclusion principle, requiring an antisymmetric wave function which had the right qualitative features for a stable molecule with a pronounced minimum in the potential energy at approximately the correct internuclear distance with approximately the right dissociation energy. More refined approximations gave a more accurate energy and equilibrium internuclear distance for the hydrogen molecule, and more radical approximation procedures brought other molecules within the purview of the methodology.

In the early days, the approximation procedures were severely restricted by the technological feasibility of performing long calculations. In the 1930s, Hartree relied on his father to do his sums. The first all-electron ab initio calculation after James and Coolidge's refinements for the hydrogen molecule in 1933 was carried out for the nitrogen molecule (Scherr 1955) with desk calculators. Performed with the help of assistants, the work took 2 years to complete. Eleven years later, Mulliken reported in his Nobel lecture that the same computation could be done in 2 min with the largest available computers! Needless to say, the advent of superfast computers with large memories revolutionized the subject, and their use was well established by the cutoff time for Gavroglu and Simões's study. Samuel Boys was an early visionary whose "unsuccessful career" (227) Coulson explained as a result of his ignoring scientific fashions and resolutely pursuing his agenda of implementing ab initio calculations at a time when the technological resources were not up to the task.

Throughout this period, the status of the subdiscipline within the experimental science of chemistry was controversial. I well remember from my own student days in the late 1960s that the assessments of the value of quantum chemistry that I heard from my experimentally minded teachers as often as not cast aspersions on the usefulness of the subject. In this connection, it is interesting to note what Stephen Brush says about his own feelings as a student of Coulson's in the 1950s. Although Brush is known for advocating the value of accommodation and not allowing scientific worthiness to hang exclusively on predictive success, he "abandoned quantum chemistry in the late 1950s because of dissatisfaction with the scientific value of the results obtained by MO calculations" (Brush 1999, 79), stressing the paucity of falsifiable claims at the time. Back in 1971, Ronald Hoffman's advocacy of "interpretive theoretical chemistry" (254) may seem to have been making a virtue of necessity. But the Woodward–Hoffman rules from the 1960s for predicting the course of organic reactions on the basis of orbital symmetry earned him the 1981 Nobel prize because of their empirical success, and he can still be heard speaking in the same vein. About this time, the tide began to turn and reasonably clean predictions (not subsequently doctored by appeal to the “flexibility” of the theory to match the data—cf. Brush 1999, fn. 68) were fulfilled. In 1965, cyclobutadiene, for example, was synthesized and shown in the late 1970s to have a rectangular structure, confirming the MO prediction of its nonaromatic character. These days, the reliability of the methods of quantum chemistry is such that they provide a means of obtaining results “unreachable by traditional experimental means” (242). But in the early days, the motivation must have relied heavily on the value of explanation and understanding.

This is readily comprehensible, even if the difficulties of prediction make it anything but straightforward. Notions of atoms were paradoxical on classical conceptions of matter. Even as the relevant atomic constituents were distinguished and their role discerned, Lewis had to stab in the dark and postulate that Coulomb’s law did not apply over atomic distances (52). Otherwise, the constituents would fly apart and atoms could not possibly provide the foundations of stable substances. Heitler and London’s paper, although only giving a rough quantitative account of the simplest case of a covalent bond, showed how a pair of particles with the same charge could actually combine to form an attractive force holding the molecule together when their behavior is understood in the light of quantum mechanical principles, in particular the near unintelligible principle of the indistinguishability of fermions.

Not wanting to let the abstruse notions get the upper hand, however, Pauling fashioned his valence bond (VB) approach which sought to preserve as much as possible of the presuppositions of structural theory that had been built up over nearly a century into a solid body of knowledge. Lewis had appraised this theory in no uncertain terms:

> No generalization of science, even if we include those capable of exact mathematical statement, has ever achieved a greater success in assembling in simple form a multitude of heterogeneous observations than this group of ideas which we call structural theory. (Lewis 1923, 20–21; quoted from the Dover edition).

Pauling wanted in particular to preserve the idea that atoms are there in the molecules, held together by bonds. But, so the story goes, as the power of computers transformed (or realised Boys’) ideas about the feasibility of extensive calculations, the molecular orbital (MO) theory championed by Mulliken came into favour. Sutcliffe paints a rather different picture, however, giving the impression that calculations based on the VB approach were always intractable:

> almost none used … the so-called valence bond (VB) approach … that Pauling had proposed as the foundation of the theory of the bond. … The nonorthogonality between the hybrid orbitals, a feature essential to the justification of the Pauling approach, made formulating the equations for calculation just too complicated and difficult, and even if approximations were made … any consequent calculations were impossible to perform. It was thus not possible to provide a means of tying Pauling’s ideas to the detailed equation in any unambiguous way. … almost all went the way that Mulliken

> proposed using a molecular orbital approach … [which made it] possible to formulate the equations in a manner suitable for calculation and to develop consistent approximation schemes that allowed at least semiempirical calculations to be made (Sutcliffe 1996, 650).

This assessment of the VB approach is much harsher than that of Gavroglu and Simões, and it would be interesting to hear their reaction to it and whether they think it fair.

Another motivating idea, especially for the early workers in the field who were trained as physicists, was the promise of a reduction of chemistry to the principles and laws of physics. The program was famously set out by Dirac, who claimed the general principles had been laid bare and it remained to carry out the difficult approximative arguments, since analytical solutions were out of the question, and show how all of chemistry is encapsulated in what would therefore merit the title of fundamental principles. Gavroglu and Simões clearly bring out this theme. But it is a great pity that they cut off their coverage in the 1970s because it was in this decade that a most interesting challenge to the reductionist thesis was raised by Guy Woolley and Brian Sutcliffe. Woolley's contribution to a section of a 1977 symposium devoted to philosophical issues gets a mention in a footnote (285), and some of his later papers are mentioned in the bibliography. But the important challenge to the presupposition of Dirac's reductionist thesis that the quantum chemists' methods yield approximations to the exact solutions and are therefore implicit in, or in some reasonable sense derived from the purely quantum mechanical principles, is not mentioned. Woolley and Sutcliffe (see especially Sutcliffe 1993) argue that the notion of molecular structure which forms the basis of chemists' reasoning about the properties and reactions of chemical substances does not in general conform to the symmetry constraints of what would be the reducing Schrödinger equation. This is a problem about which Per-Olov Löwdin—a prominent figure in Gavroglu and Simões's book—worried about towards the end of his life in a number of papers investigating the quantum mechanical definition of a molecule. However, whereas Löwdin believed that molecular symmetry must be somehow contained in the Coulombic Hamiltonian, though he knew not where or how, Woolley and Sutcliffe think it not at all evident that the Coulombic Hamiltonian alone gives rise to the chemically interesting features of molecules. Rather, they think that molecular structure is, in their words, "put in by hand", that is, introduced on the basis of additional, independent assumptions which, taken together with quantum mechanics, form a foundation for molecular structure adequate for chemistry. Sutcliffe (1996) points out that Berry had already called attention to the way the Born–Oppenheimer assumption puts aside the permutation symmetry of the nuclei (Berry 1960). But their efforts do not seem to have attracted much attention from either the physics or the chemistry community, and they say (somewhat reminiscent of Boys' experience) that this work has not done their careers any good.

Woolley and Sutcliffe's argument addresses the physicists' conception of reduction on its own terms. Gavroglu and Simões emphasize the other side of the coin, the chemists' perspective. The chemists' way of doing things is not the same as the physicists'. "Different scientific communities", they say, "impose different explanatory demands on their theories, and this constitutes an important cultural characteristic of each community" (258). This echoes points made in the philosophical literature in criticism of Nagel's classic conception of reduction as deduction of the reduced theory from the reducing theory together with bridge laws. Sciences such as biology and psychology, so the argument goes, do not have the same deductive character that has been taken to be characteristic of physics, which renders the Nagelian model inapplicable (see, e.g., Kitcher 1984). Any talk of reduction must accommodate the manner of theory construction and explanatory strategies characteristic of these disciplines rather than seeking to impose a structure which is foreign to the putatively reduced discipline. Such an imposition lacks motivation independent of the anticipated reduction. In fact, if chemists had not been able to point the physicists in the right direction, it is anybody's guess where they might have got to in relating chemistry to physics at the microlevel. As Kohler (1971, 344) put it, "without the idea of the shared bond, … the application of quantum mechanics to the chemical bond in the late 1920s by H. [*sic*] London, E. Schrödinger, and L. Pauling would have begun on far less certain ground". The question is whether it would have begun at all.

Gavroglu and Simões go some considerable way to showing how the spirit of chemical research has been taken on board by the quantum chemists. However, there is one aspect of the tale that I missed. Chemistry is "concerned", as a prominent organic chemist puts it, "with substances and with their transformations into other substances" (Benfey 1963, 574). But very little is said in Gavroglu and Simões's book about this latter aspect, the transformation of substances, or in more modern jargon, the nature of chemical reactions. In particular, no mention is made of transition state theory first developed by Eyring and coworkers in the 1930s. Just as quantum chemists strove to retain as much as possible from classical structure theory in their theories of molecular structure, transition state theory sought to build on classical ideas in kinetic theory on the role of activation energy and collision frequency governing the rate of chemical reactions. As with the theory of molecular structure, the principal contribution of the theory was to the understanding of the mechanisms of chemical reactions underlying the observed reaction kinetics and its response to varying circumstances rather than precise quantitative predictions (Laidler and King 1983). But the theory involved the application of quantum mechanical principles to the interpretation and development of the Arrhenius equation, covering a central area of chemistry and falling squarely within the scope of Gavroglu and Simões's book with regard to both subject matter and historical period.

There will always be someone who finds some aspect or other lacking from a book. Nothing said here is intended to detract from the judgment that Gavroglu and Simões have done an excellent job in mastering a large body of material which they have brought to life by their organizational themes. There are many aspects of Gavroglu and Simões's book which have not been taken up here, but which will be of interest to historians and philosophers concerned with the development of modern chemistry. I expect such people will find it every bit as rewarding to read as I have.

Authors' response: Kostas Gavroglu and Ana Simões

Lucky are the authors whose books are read carefully and critically. We are both lucky and thankful that three scholars with outstanding contributions in their related fields have been such careful and thorough readers of our book, have shown us some of its weak parts, have pointed out a number of issues for further discussion, and, at the same time, have been so generous in their specific and overall assessments. We are deeply obliged to them. Each of the reviewers has emphasized different aspects of our work, and, thus, we have greatly benefited from this wide spectrum of analyses which, also, reflects their scholarly contributions. Each reviewer approached the book from a different perspective. Hasok Chang's work has been underlining the great possibilities provided by a unified approach to history and philosophy of science, Jeremiah James has been beautifully combining history of science with science studies, and Paul Needham's work has been raising over the years a series of intriguing philosophical issues in relation to the nitty–gritty aspects of chemistry.

Though we fully realize that there are many and good reasons to subscribe to the "end of disciplines" to which many historians of science—including Jeremiah James—have adhered to recently, there is still a lot to be learned from writing such disciplinary histories. We, still, insist that throughout the twentieth century the great majority of scientists have been almost exclusively involved with establishing and legitimizing disciplines. The intense academic fights over the establishment of departmental positions, the foundation of new journals, the funding of research, the organization of conferences, the establishment of new societies or new branches within more traditional societies, the new kinds of textbooks, book series, etc., comprise a substantial part of the social dynamics which have brought about the specific characteristics of disciplines. This, in fact, is contingency at its best: things, indeed, could have developed differently, but they developed the ways they did because specific scientists had chosen specific strategies to articulate and legitimize "their" disciplines. Hence, our insistence to write a disciplinary history has been partly conditioned by the need to capture the differing yet converging efforts of all those who have been insisting that they aimed at establishing a discipline and through a series of complex processes—conceptual as well as social—gave the discipline its own particular characteristics. Our story is surely not the whole story, but it is also the case that whatever the whole story may be, it cannot be narrated by ignoring this particular viewpoint.

Our emphasis on an "in-between" discipline such as quantum chemistry does not imply that quantum chemistry was in a state of limbo. Quite the opposite was the case: The original fluid state gave way to a rather impressive stability, not because there was a consensus around the paradigm to be adopted by the relevant community, but because the issues related to its identity—methodological, conceptual, technical, institutional—through continuous reconceptualizations and negotiations at the core of everyday practices, became in the end part of a culture whose strength derived from its ability to accommodate diversity, much like the different strands of an artificial fiber gain strength through the interlocking of its diverse elements, according to Coulson's telling metaphor.

In our book, the development of an “in-between” discipline such as *quantum chemistry* is narrated through six interrelated clusters of issues that manifest the particularities of its evolving (re)articulations with chemistry, physics, mathematics, and biology, as well as its institutional positioning. The first cluster involves issues related to the historical becoming of the epistemic aspects of *quantum chemistry*: the multiple contexts that prepared the ground for its appearance; the ever present dilemmas of the initial practitioners as to the “most” appropriate course between the rigorous mathematical treatment, its dead ends, and the semiempirical approaches with their many promises; the novel concepts introduced and the intricate processes of their legitimization. Though it may appear that there was a consensus that *quantum chemistry* had always been a “branch” of chemistry, this was not so during its history, and different (sub)cultures (physics, applied mathematics) attempted to appropriate it. The historical development of *quantum chemistry* has been the articulation of its relative autonomy both with respect to physics as well as with respect to chemistry, and we argue for the historicity of this relative autonomy. The second cluster of issues is related to disciplinary emergence: the naming of chairs, university politics, textbooks, meetings, networking, as well as alliances the practitioners of the new discipline sought to build with the practitioners of other disciplines were quite decisive in the formation of the character of *quantum chemistry*. The third cluster of issues is related to the contingent character of *quantum chemistry*. *Quantum chemistry* could have developed differently; the particular form it took was historically situated, at times being the result of not only technical but also cultural and philosophical considerations. What is important to understand is not what different forms *quantum chemistry* could or might have taken, but, rather, the different possibilities open for developments and the difficulties that at each particular historical juncture formed barriers that dissuaded practitioners from pursuing these possibilities. Throughout this 50-year period, the criteria for assessing the “appropriateness” of each approach being developed gravitated among a rigorous commitment to quantum mechanics, a pledge toward the development of a theoretical framework where quasi-empirical outlooks played a rather decisive role in theory building, and a vow to develop approximate techniques for dealing with the equations. Such criteria were not, strictly speaking, solely of technical character, and the choices adopted by the various practitioners at different times had been conditioned by methodological, philosophical, and ontological commitments and even by institutional considerations. The fourth cluster of issues is related to a rather unique development in the history of *quantum chemistry*: The rearticulation of the practices of the community after the early 1960s, which was brought about by one artifact—the electronic computer. Calculations, which had been impossible to perform, appeared at long last to be manageable! The fifth cluster of issues is related to philosophy of science. The issues that have been raised throughout the history of *quantum chemistry* played a prominent role in philosophical elaborations and discussions of reductionism, scientific realism, the role of theory, including its descriptive or predictive character, the role of pictorial representations and mathematics, the role of semiempirical versus ab initio approaches, and the status of theoretical entities and of empirical observations. The sixth cluster is of a quasi-methodological and quasi-cultural character. The history of *quantum chemistry* displays instances that we approach in terms of "styles of reasoning."

Glancing at the classification table by the European Research Council and excluding those entries for Engineering and the Life Sciences we come up with a long list of disciplines (mostly "in-between" just like quantum chemistry). Here are some examples: Astrobiology, atmospheric chemistry, atmospheric physics, biogeochemistry, biogeography, biological chemistry, biomaterials, biophysics, chemical oceanography, chemical physics, colloid chemistry, electrochemistry, environment chemistry, geochemistry, geomagnetism, nuclear chemistry, photochemistry, physical chemistry, physical geography, radiation chemistry, surface science, terrestrial ecology, etc. Now if we replace the italicized "quantum chemistry" in the above paragraph with any of these disciplines, what applies to quantum chemistry appears to be equally relevant to the history of each one of them—some of which are still lacking even a simple chronology of their development! Thus, it might be the case that these six clusters of issues—the epistemic content of a subdiscipline, the social processes involved in disciplinary emergence, the contingent character of its various developments, the dramatic changes brought about by the digital computer, the philosophical concerns of the protagonists, and the importance of styles of reasoning in assessing different approaches to the becoming of a particular subdiscipline—may form a framework for weaving the narrative strands of the history of various in-between disciplines. Surely there is much more to their history, surely the history of disciplines is not the whole story, but surely an important part of the history of science can be understood through disciplinary history. Let us stress that this is neither a prescription of how to do disciplinary history nor an algorithm to be applied for every different discipline nor is the case that each one of these clusters are equally suggestive for understanding the history of every discipline.

A theme that all three reviewers underline is the relevance of a number of comments we made on philosophical and methodological issues. It is, indeed, the case that we have made an effort to discuss the ways some of the problems that appear in philosophy of science (and, in particular, in philosophy of chemistry) were being articulated within the context of the history of quantum chemistry. Needless to say that the relatively recent efforts by well-known historians as well as philosophers of science to reset the agenda of an integrated history and philosophy of science have been quite decisive for the ways we discussed these issues. Hasok Chang, who has been so committed to this venture, has chosen to highlight those points in our book in an especially generous way.

There is, in particular, one consideration that we have realized by reading the reviews which we would like to discuss. Writing the history of a discipline is writing about the becoming of a culture specific to that discipline. Throughout the intricate processes of legitimation of (any) in-between discipline, the ideas, practices, institutions, and their interrelationships form the culture (with its associated subcultures) of those who identify themselves as constituting the community of practitioners of that particular discipline. It seems that a host of philosophical issues have a different relevance for and are expressed in different terms by different disciplinary cultures. Issues in philosophy of science have often been debated as if they have an exclusive reference to physics, and since physics is considered as the scientific field *par excellence,* the philosophical discussions are presented as having a transdisciplinary scope. A host of discussions concerning philosophical issues in the sciences rely on the assumption that there is a hierarchy among the sciences, physics being at the "top" of this hierarchy. In this book, we have tried to explore another approach. Perhaps philosophical issues should not even be considered as "belonging" to a discipline as such, but to its practitioners, since it is the discourse *they* form that accommodates these issues. By attempting to study the possibilities provided by such an approach, we tried to historicize the philosophical problems appearing in quantum chemistry. During the process of delineating a (new) in-between discipline, those who play any role in its becoming do not only devise and appropriate ideas, techniques and practices, but *contextualise philosophical problems* in order to make additional differentiations with respect to the parent disciplines. As we argue in the book, the whole problem of reductionism is on a totally different footing when discussed within the context of (quantum) chemistry than it is the case when discussed within physics. The same holds true when (quantum) chemistry forces us to dramatically reassess the role of theory and its relations to experiment. This is why it may be interesting to have more disciplinary histories and test the extent that they may be useful probes for revealing different contextualizations of issues in the philosophy of science.

In discussing the philosophical issues of quantum chemistry, it would not be right to put all the emphasis on the question of reductionism. The question of realism has, also, been intensely discussed by quantum chemists, since coming to a consensus concerning the ontological status of a number of entities (resonance being one among others) was dictated by practical necessities and not by philosophical sensitivities. Let us remember that for many decades chemists considered chemistry as an exclusively laboratory science. And when there were the first attempts at the end of the nineteenth century to adopt a "theory" for chemistry, whether that was the chemical thermodynamics as developed by van 't Hoff or the various mathematical models for the structure of the atoms and the various forces between and within atoms, or to subscribe to models explaining the differences between the physical and chemical atom, the chemists gave a strong and obstinate fight to stick to their exclusively laboratory science. Concentrating on the period after the advent of quantum mechanics, it is our feeling that chemists dealt with the conceptual difficulties of their discipline in a manner that was rather different from the ways physicists did. Physicists are rather used to working with abstract entities, and the questioning (by them or by philosophers) of the ontological status of these entities is not something which comes as a surprise to them. It has become part of their culture. Even if a number of physicists were willing to acknowledge the existence of these problems, such an acknowledgment did not interfere with their everyday practices; they continued happily with their calculations and experiments. Some physicists were willing to hear the views of the philosophers of science who studied these problems. Few were willing to intervene in these discussions. Not so with the chemists. Throughout the history of quantum chemistry, chemists never shied away when they came in contact with a philosophical problem. Interestingly, what we consider as a philosophical problem, to chemists was a "real" problem, which they had to deal with. They discussed it as chemists, and though a realization of such problems did not block their going on with their calculations and experiments, there was a widespread feeling that these are issues that they—as practicing chemists—had to come to grips with. In our book, we have many such examples. Perhaps, this may be one of many parameters which may explain the late rise of philosophy of chemistry: Chemists collectively did not delegate the discussion of these kinds of problems to others as the physicists did. And, perhaps, this active involvement of chemists in the philosophical issues of their discipline may, also, account for the great success of philosophy of chemistry.

The suggestion for a glossary made by Hasok Chang is correct, and we hope to be able to include one in a possible second edition. Jeremiah James and Paul Needham have pointed out that we should have presented the Born–Oppenheimer approximation, or, even, the transition state theory first developed by Henry Eyring and co-workers in the 1930s. We consciously did not include many such aspects of the history of post-1926 chemistry, since our project would have been totally unmanageable. Nevertheless, we should have mentioned what we leave out and justify the reasons for such omissions. But, most importantly, we decided to keep clear of all the discussions on quantum mechanics *per se*, which were taking place in the 1930s when quantum chemistry was also starting to achieve its autonomy. We have refrained from bringing into the discussion the views of many physicists about quantum mechanics and/or chemistry, and we preferred to look at quantum mechanics almost exclusively from the chemists' point of view, even if some of our protagonists had a background in physics.

It may, however, be of interest to comment on the issue of the Born–Oppenheimer approximation. There were discussions involving many physicists and quantum chemists, including Philip Anderson, Hans Primas, R. G. Woolley, S. J. Weininger, and Brian T. Sutcliffe, as to the impossibility of deriving the notion of molecular structure from Schrödinger's equation without the Born–Oppenheimer approximation. This has been a lively and fascinating topic, to which we did not refer, not primarily due to restrictions imposed by the time frame of our narrative, but due to the perspective we adopted, namely to discuss the issue of reductionism from the point of view of chemists and not of physicists. It appears that chemists have not shown any particular concern for justifying the Born–Oppenheimer approximation, having taken for granted the chemical notion of molecular structure inherited from classical structure theory. Going a step further, we agree with Sutcliffe when he says, in a recent review of our book (*HYLE*, 18:1, May 2012, 91–4), that even if chemists were aware of the implications of these discussions they would probably continue to ignore them, as they do at present. This is not to imply that chemists are indifferent to such questions, but that the culture which binds them together is not too permissive toward such discussions. Is this not, after all, another striking instance of the power of cultural factors constraining committed practitioners?

Finally, there are a number of interesting points raised by Needham, referring to quantum chemistry after the mid-1970s when we decided to end our story. We would like to comment on one of them, that is, the status of the valence bond (VB) approach of Linus Pauling after the development of computer programs that were extensively used for the solution of chemical problems. It is certainly the case that the molecular orbital (MO) approach initiated by Friedrich Hund and Robert Sanderson Mulliken turned out to be particularly convenient when the possibility to deal with various problems in quantum chemistry through the use of computers arose in the 1970s. But, as we argue throughout our book, the two approaches differed in many respects and most significantly on how they considered quantum chemistry to acquire a theory of "its own." So, what was in the minds of a lot of quantum chemists was not getting results in exclusion of anything else, but getting results within the theoretical framework which was—methodologically, philosophically, and ontologically—more appealing to them. How the new consensus around the MO approach was achieved is an interesting story, which goes beyond the fact that one could get better results through its use in computer programming—though this was an important factor. Suffice it to remember that Roy McWeeny, the supervisor of Sutcliffe, cited by Needham on this issue, continued to explore the VB approach, trying to counteract the received view according to which it was not amenable to ab initio calculations.

Authors do not have always the opportunity to respond to the critical comments of reviewers. We had such an immensely stimulating and rewarding chance, and we heartily thank the editors of *Metascience*—Theodore Arabatzis and Stathis Psillos—for providing us with such an occasion.

References

Arabatzis, T. 2006. *Representing electrons: A biographical approach to theoretical entities*. Chicago: University of Chicago Press.

Benfey, O.T. 1963. Concepts of time in chemistry. *Journal of Chemical Education* 40: 574–577.

Berry, R.S. 1960. Time-dependent measurements and molecular structure: Ozone. *Reviews of Modern Physics* 32: 447–454.

Brush, S. 1999. Dynamics of theory change in chemistry: Benzene and molecular orbitals, 1945–1980. *Studies in History and Philosophy of Science* 30: 263–302.

Chandler, J. and A. Davidson (eds). 2009. The fate of disciplines. *Critical Inquiry* 35(4): 729–1053.

Daston, L. 2009. Science studies and the history of science. *Critical Inquiry* 35: 798–813.

de Chadarevian, S. and H.-J. Rheinberger (eds). 2009. Disciplinary histories and the history of disciplines: The challenge of molecular biology. *Studies in the History and Philosophy of Biological and Biomedical Sciences* 40(1): 1–72.

Galison, P. 2004. Mirror symmetry: Persons, values, and objects. In *Growing explanations*, ed. M.N. Wise, 23–63. Durham: Duke University Press.

Gibbons, M., C. Limoges, H. Nowotny, S. Schwartzman, P. Scott, and M. Trow. 1994. *The new production of knowledge*. London: Sage.

Kitcher, P. 1984. 1953 and all that: A tale of two sciences. *Philosophical Review* 93: 335–373.

Kohler Jr., R. E. 1971. The origin of G. N. Lewis's theory of the shared pair bond. *Historical Studies in the Physical Sciences* 3: 343–376.

Kuhn, T.S. 1962. *The structure of scientific revolutions*. Chicago: University of Chicago Press.

Laidler, K.L., and M.C. King. 1983. The development of transition-state theory. *Journal of Physical Chemistry* 87: 2657–2664.

Latour, B. 1987. *Science in action*. Cambridge: Harvard University Press.

Lemaine, G., R. MacLeod, M. Mulkay, and P. Weingart, eds. 1976. *Perspectives on the emergence of scientific disciplines*. Paris, Chicago: The Hague.

Lenoir, T. 1997. *Instituting science: The cultural production of scientific disciplines*. Stanford: Stanford University Press.

Lewis, G. N. 1923. *Valence and the structure of atoms and molecules.* Washington, DC: Chemical Catalogue Company; reprinted by Dover, New York, 1966.

Nye, M.J. 1992. Physics and chemistry: Commensurate or incommensurate sciences? In *The invention of physical science*, ed. M.J. Nye, J. Richards, and R.H. Stuewer, 205–224. Dordrecht: Kluwer.

Nye, M.J. 1993a. National styles? French and English chemistry in the nineteenth and early twentieth centuries. *Osiris* 8: 30–49.

Nye, M.J. 1993b. *From chemical philosophy to theoretical chemistry*. Berkeley: University of California Press.

Scerri, E.R. 2008. *Collected papers on philosophy of chemistry*. London: Imperial College Press.

Scherr, C.W. 1955. An SCF LCAO MO study of N_2. *Journal of Chemical Physics* 23: 569–578.

Sukumar, N. 2009. The chemist's concept of molecular structure. *Foundations of Chemistry* 11: 7–20.

Sutcliffe, B.T. 1993. The coupling of nuclear and electronic motions in molecules. *Journal of the Chemical Society, Faraday Transactions* 89: 2321–2335.

Sutcliffe, B.T. 1996. The development of the idea of a chemical bond. *International Journal of Quantum Chemistry* 58: 645–655.