Em reconhecimento das suas contribuições importantes na área, a tónica dos capítulos que amigos e colaboradores de António Amorim da Costa trazem a este livro vai desde facetas da história da ciência relacionadas com a química e da sua pré-história, através da alquimia, a iatroquímica, o período do flogisto, a química pneumática e finalmente a história da química quântica e mecânica estatística em tempos mais próximos do nosso. Há uma ênfase muito particular nos aspectos históricos do desenvolvimento da química em Portugal e no Brasil.

No entanto a química não se desenvolveu de forma isolada, e as contribuições para este livro abordam áreas adjacentes, como a electricidade, a medicina, a óptica e a mineralogia. Além disso, a história não lida apenas com factos. Diz respeito também a pessoas, como o Luso-Brasileiro do século XVIII, o engenheiro José Fernandes Pinto Alpoim, ou o químico português do século XIX Professor de química da Universidade de Coimbra Thomé Rodrigues Sobral, e muitos mais. Desejamos que estes "pedaços" da história das ciências venham enriquecer a nossa compreensão e reconhecer as contribuições feitas por António Amorim da Costa para a área.
IX.

ASPECTS FROM THE HISTORY OF QUANTUM CHEMISTRY

We have known António Amorim da Costa since the late 1990s, as we have been participating in the multinational project “The Evolution of Chemistry in Europe, 1789–1939” funded by the European Science Foundation (ESF). A physical chemist, Amorim da Costa became interested in the history of science in the late 1970s and has been contributing talks, papers and books, especially focusing on the history of chemistry in Portugal, addressed to lay and specialized audiences.¹ His initial historical interest fell on the history of chemistry at the reformed University of Coimbra, its professors, ideas and practices, and their reactions to the chemistry of Lavoisier. He collaborated in the organization of the meeting on “Revolutions in Science” in Coimbra in 1986, and together with William Shea and the late Alan Debus, contributed to foster the discipline of the history of science in Portugal in the late 1980s and early 1990s.² For both of us who are actively involved in the further consolidation of the discipline in our respective countries, we know how difficult it should have been to take such initiatives and Antonio took. He, also, participated in the commemorative volumes celebrating the 200th anniversary of the Academy of Sciences of Lisbon, again offering reflections on 18th century chemistry in Portugal.³ His contributions to the history of science were extended to other periods, especially as a participant in the ambitious ESF project on the history of chemistry, in which he offered the international community his assessment of the role of chemistry in Portugal in late 19th and early 20th centuries.⁴ An active physical chemist who became a scientist-historian, Amorim da Costa has been also very supportive of the
younger generation of professional historians of science in our respective countries, showing a rare gift for interacting with all of us. We are truly thankful to him.

Although we could have contributed to this volume with a discussion of the appropriation of the new sciences in the European periphery during the 18th century, a topic to which we have both contributed and which is akin to the historical area which Amorim da Costa selected for his initial steps as a historian, we opted to offer our more recent reflections on the history of quantum chemistry, for two reasons. The first time the authors of this chapter both met with Amorim da Costa happened to be at the meeting of the ESF in Delphi, Greece, and following this meeting we contributed to the ESF project with a paper on textbooks in the history of quantum chemistry. Second, the history of quantum chemistry is probably a topic more appealing to many of those who will be reading this volume. We hope to present some of the new vistas the history of chemistry has to offer.

In 1969 in a symposium on the “Fifty Years of Valence” Charles Alfred Coulson, the writer of the well known textbook titled *Valence*, then Professor of Applied Mathematics at the University of Oxford, was emphatically declaring that one of the primary tasks of the chemists during the initial stage in the development of quantum chemistry was to *escape from the thought forms of the physicists.* Indeed. Among the many and, at times, insurmountable barriers during the becoming of quantum chemistry, perhaps the one hurdle that was the most incapacitating was the danger to develop a subdiscipline in chemistry that would be indistinguishable from a subdiscipline in physics. Hence, escaping the thought forms of the physicists was a strategic choice – not by all the protagonists, not even consciously pursued, but, surely, in the minds of those whose work eventually established quantum chemistry.

In 1927 Walter Heitler and Fritz London by using the then newly proposed Schrödinger equation, calculated the strength of the homopolar bond of the hydrogen molecule. They were able to show in no uncertain terms that the homopolar bond – a kind of mystery within the classical framework – could be mathematically tackled and physically understood by using the