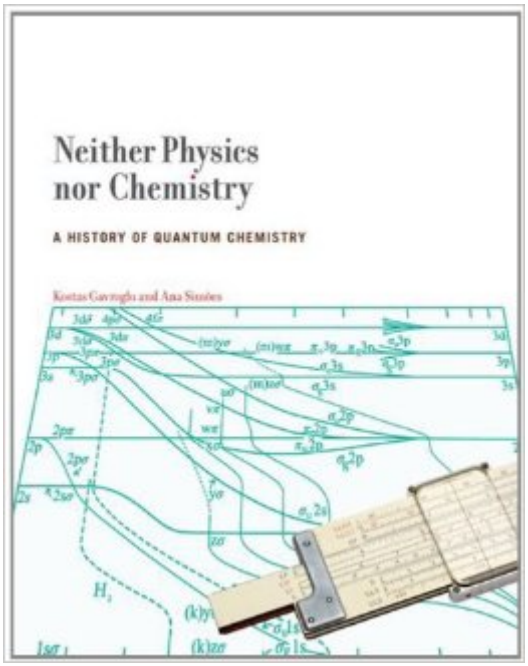
# Neither Physics Nor Chemistry: A History Of Quantum Chemistry (Transformations: Studies In The History Of Science And Technology)



## Synopsis

Quantum chemistry--a discipline that is not quite physics, not quite chemistry, and not quite applied mathematics--emerged as a field of study in the 1920s. It was referred to by such terms as mathematical chemistry, subatomic theoretical chemistry, molecular quantum mechanics, and chemical physics until the community agreed on the designation of quantum chemistry. In Neither Physics Nor Chemistry, Kostas Gavroglu and Ana SimÃ  es examine the evolution of quantum chemistry into an autonomous discipline, tracing its development from the publication of early papers in the 1920s to the dramatic changes brought about by the use of computers in the 1970s. The authors focus on the culture that emerged from the creative synthesis of the various traditions of chemistry, physics, and mathematics. They examine the concepts, practices, languages, and institutions of this new culture as well as the people who established it, from such pioneers as Walter Heitler and Fritz London, Linus Pauling, and Robert Sanderson Mulliken, to later figures including Charles Alfred Coulson, Raymond Daudel, and Per-Olov LÃ¶wdin. Throughout, the authors emphasize six themes: epistemic aspects and the dilemmas caused by multiple approaches; social issues, including academic politics, the impact of textbooks, and the forging of alliances; the contingencies that arose at every stage of the developments in quantum chemistry; the changes in the field when computers were available to perform the extraordinarily cumbersome calculations required; issues in the philosophy of science; and different styles of reasoning.

## Book Information

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## Customer Reviews

This book presents the first in-depth historical analysis of quantum chemistry, a field that according to the title is neither physics nor chemistry. I am not sure how many practicing quantum chemists will agree on this view point, nevertheless the authors provide compelling support for their thesis. Soon after the advent of quantum mechanics (QM) in 1925, Walter Heitler and Fritz London wrote a landmark paper where they expounded the first quantum mechanical treatment of the chemical bonding in the hydrogen molecule (H2). Soon after many talented physicists and chemists joined the field and two competing theories took shape: on the one side the valence bond (VB) theory of Heitler-London-Slater-Pauling and on the other the molecular orbital (MO) theory of Mulliken and Hund. Applied mathematicians (Coulson, Hartree, and later on Pople) also contributed greatly to this new field along with many other colleagues from Europe, US, and Japan. In 1967, the Swedish physicist Per-Olov Lowdin established the International Journal of Quantum Chemistry (IJQC) which represented an important step toward the consolidation of this scientific discipline.The authors, both professional historians of Science, explain in great detail all the intricacies connected with the theoretical formulation of the above VB and MO theories, starting from the pre-QM work of Gilbert Lewis on the electron pair concept that appeared in 1916 up to the early 1970s when computers (mainframes) became available to many research groups around the world. There are, however, some important details that they left out as practicing computational quantum chemists will notice.

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