

Joachim Reinhold

# Quantentheorie der Moleküle

Eine Einführung

*5. Auflage*



Springer Spektrum

# Quantentheorie Und Chemie

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## **Quantentheorie Und Chemie:**

*Quantentheorie und Chemie* Hans Falkenhagen,1928      *Neither Physics nor Chemistry* Kostas Gavroglu,Ana Simoes,2011-10-07 The evolution of a discipline at the intersection of physics chemistry and mathematics 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 Simoes 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 Löwdin 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      *The Collected Works of P. A. M. Dirac: Volume 1* P. A. M. Dirac,1995-10-26 A comprehensive collection of the scientific papers of one of this century's most outstanding physicists      **Histories of the Electron** Jed Z. Buchwald,Andrew Warwick,2004-01-30 A biography of the electron and a history of the microphysical world that it opened up      **Molecular Interaction Fields** Peter W. Atkins,2006 This unique reference source edited by the world's most respected expert on molecular interaction field software covers all relevant principles of the GRID force field and its applications in medicinal chemistry Entire chapters on 3D QSAR pharmacophore searches docking studies metabolism predictions and protein selectivity studies among others offer a concise overview of this emerging field As an added bonus this handbook includes a CD ROM with the latest commercial versions of the GRID program and related software      *Erich Hückel (1896-1980)* Andreas Karachalios,2009-12-08 This comprehensive account of Hückel's career examines his scientific work and his key role in the emergence of quantum chemistry as an independent discipline It also covers his clash with Linus Pauling over the properties of the benzene molecule      *"The" Conceptual Completion and the Extensions of Quantum Mechanics 1932 - 1941 ; Epilogue: Aspects of the Further Development of Quantum Theory 1942 - 1999* Jagdish Mehra,Helmut Rechenberg,2001-06-29 Quantum Theory together with the principles of special and general relativity constitute a scientific revolution that has profoundly influenced the way in which we think about the universe and the fundamental forces that govern it The Historical Development of

Quantum Theory is a definitive historical study of that scientific work and the human struggles that accompanied it from the beginning Drawing upon such materials as the resources of the Archives for the History of Quantum Physics the Niels Bohr Archives and the archives and scientific correspondence of the principal quantum physicists as well as Jagdish Mehra s personal discussions over many years with most of the architects of quantum theory the authors have written a rigorous scientific history of quantum theory in a deeply human context This multivolume work presents a rich account of an intellectual triumph a unique analysis of the creative scientific process The Historical Development of Quantum Theory is science history and biography all wrapped in the story of a great human enterprise Its lessons will be an aid to those working in the sciences and humanities alike Comments by distinguished physicists on The Historical Development of Quantum Theory the most definitive work undertaken by anyone on this vast and most important development in the history of physics Jagdish Mehra trained in theoretical physics under Pauli Heisenberg and Dirac pursued the vision of his youth to write about the historical and conceptual development of quantum theory in the 20th century This series of books on the HDQT has thus become the most authentic and permanent source of our knowledge of how quantum theory its extensions and applications developed My heartfelt congratulations Hans A Bethe Nobel Laureate A thrilling and magnificent achievement

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