Record Nr. UNINA9910781981203321 Autore Gavroglou Kostas Titolo Neither physics nor chemistry: a history of quantum chemistry / / Kostas Gavroglu and Ana Simoes Cambridge, Mass., : MIT Press, ©2012 Pubbl/distr/stampa **ISBN** 1-283-30283-7 9786613302830 0-262-29875-9 Descrizione fisica 1 online resource (367 p.) Collana Transformations: studies in the history of science and technology Disciplina 541/.28 Soggetti Quantum chemistry - History Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Description based upon print version of record. Includes bibliographical references and index. Nota di bibliografia Contents; Preface; Introduction; Chapter 1. Quantum Chemistry qua Nota di contenuto Physics: The Promises and Deadlocks of Using First Principles; The Old Quantum Chemistry: Bonds for Physicists and Chemists; Walter Heitler and Fritz London: Outlining a Program for Quantum Chemistry; Erich Huckel: Nonvisualizability and the Quantum Theory of the Double Bond; Hans Hellmann: Fundamental Theorems and Semi-empirical Approaches; Friedrich Hund: Foundations of Molecular Spectroscopy in Quantum Mechanics; Some Further Remarks; Chapter 2. Quantum Chemistry gua Chemistry: Rules and More Rules The Young Mulliken: Hinting at Molecular Orbitals Gilbert Newton Lewis: A Precursor; Linus Pauling: Exploring Different Possibilities for a Quantum Mechanical Theory of Valence; 1931: The Annus Mirabilis for Quantum Chemistry; Two Parallel Research Agendas; The Development of Mulliken's Program: What Are Electrons Really Doing in Molecules?; Playing the Devil's Advocate: Heitler and London: The Lost Battle: Legitimation through Pedagogical Considerations; Two Nobel Prizes Worlds Apart: Some Further Remarks Chapter 3. Quantum Chemistry qua Applied Mathematics:

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## Sommario/riassunto

The authors of this book 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.