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Atomic Hypothesis and the Concept of Molecular Structure

By Zvonimir B. Maksic

Springer Nov 2013, 2013. Taschenbuch. Book Condition: Neu. 242x170x19 mm. This item is printed on demand - Print on Demand Neuware - 'Imagination and shrewd guesswork are powerful instruments for acquiring scientific knowledge . . . ' 1. H. van't Hoff The last decades have witnessed a rapid growth of quantum chemistry and a tremendous increase in the number of very accurate ab initio calculations of the electronic structure of molecules yielding results of admirable accuracy. This dramatic progress has opened a new stage in the quantum mechanical description of matter at the molecular level. In the first place, highly accurate results provide severe tests of the quantum mechanics. Secondly, modern quantitative computational ab initio methods can be synergetically combined with various experimental techniques thus enabling precise numerical characterization of molecular properties better than ever anticipated earlier. However, the role of theory is not exhausted in disclosing the fundamental laws of Nature and production of ever increasing sets of data of high accuracy. It has to provide additionally a means of systematization, recognition of regularities, and rationalization of the myriads of established facts avoiding in this way complete chaos. Additional problems are represented by molecular wavefunctions provided...



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