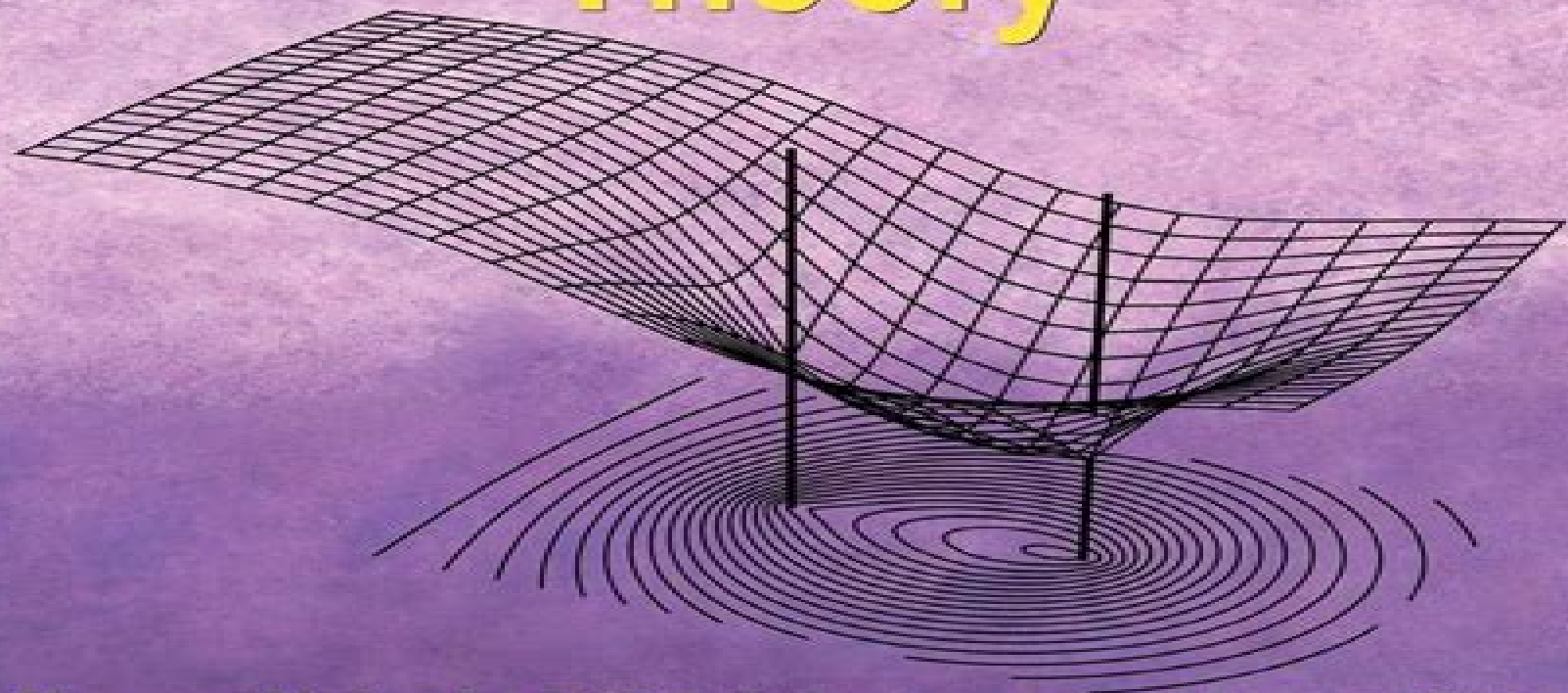


Molecular Electronic-Structure Theory



Trygve Helgaker | Poul Jørgensen | Jeppe Olsen

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Stephen Wilson, Geerd H.F. Diercksen



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Schaefer, 2004-01-01 For each of 150 landmark papers in ab initio molecular electronic structure methods, the author provides a lucid commentary. The primary focus is methodology rather than particular chemical problems. The selected papers present important methods and illustrate their effectiveness in predicting a variety of chemical phenomena. 1984 edition. *A Snapshot of Molecular Electronic Structure Theory and its Applications*, 2025-10-01 A Snapshot of Molecular Electronic Structure Theory and its Applications, Volume 92 in the Advances in Quantum Chemistry series highlights new advances in the field with this new volume presenting interesting chapters on topics such as Polynomial expression of variable precision of molecular integrals for orbital exponents and atomic distances over STO. A first step towards the development of exchange correlation functionals from X ray diffraction data. Quantum Mechanical Insights into the Properties of Graphene like Zinc Oxide g ZnO. Theoretical study of structural aspects and interactions between Ederavone and Cucurbit 7 uril. Time dependent potential models for atomic spectroscopy in atmospheric plasmas and much more. Additional chapters cover Anionic resonances of Mg and Ca from an electron propagator based on a multiconfigurational reference state and a complex absorbing potential. Massively Lockstep Parallel Algorithms for Full Isomerspace Geometry Optimization. A

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evaluation of energy derivatives from reliable wave functions can hardly be overestimated This monograph presents the formulation and implementation of analytical energy derivative methods in ab initio quantum chemistry It includes a systematic presentation of the necessary algebraic formulae for all of the derivations The coverage is limited to derivative methods for wave functions based on the variational principle namely restricted Hartree Fock RHF configuration interaction CI and multi configuration self consistent field MCSCF wave functions The monograph is intended to facilitate the work of quantum chemists and will serve as a useful resource for graduate level students of the field

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Methods in Computational Molecular Physics Stephen Wilson, Geerd H.F. Diercksen, 2013-11-11 This volume records the lectures given at a NATO Advanced Study Institute on Methods in Computational Molecular Physics held in Bad Windsheim Germany from 22nd July until 2nd August 1991 This NATO Advanced Study Institute sought to bridge the quite considerable gap which exist between the presentation of molecular electronic structure theory found in contemporary monographs such as for example McWeeny's Methods of Molecular Quantum Mechanics Academic Press London 1989 or Wilson's Electron correlation in molecules Clarendon Press Oxford 1984 and the realization of the sophisticated computational algorithms required for their practical application It sought to underline the relation between the electronic structure problem and the study of nuclear motion Software for performing molecular electronic structure calculations is now being applied in an increasingly wide range of fields in both the academic and the commercial sectors Numerous applications are reported in areas as diverse as catalysis and interstellar chemistry drug design and environmental studies molecular biology and solid state physics The range of applications continues to increase as scientists recognize the importance of molecular structure studies to their research activities Recent years have seen a growing dependence of these applications on program packages which are often not in the public domain and which may have a somewhat limited range of applicability dictated by the particular interests and prejudices of the program author

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