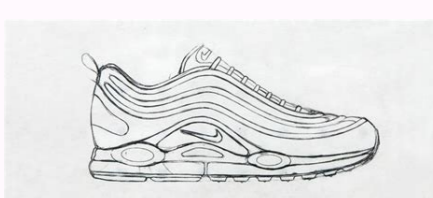
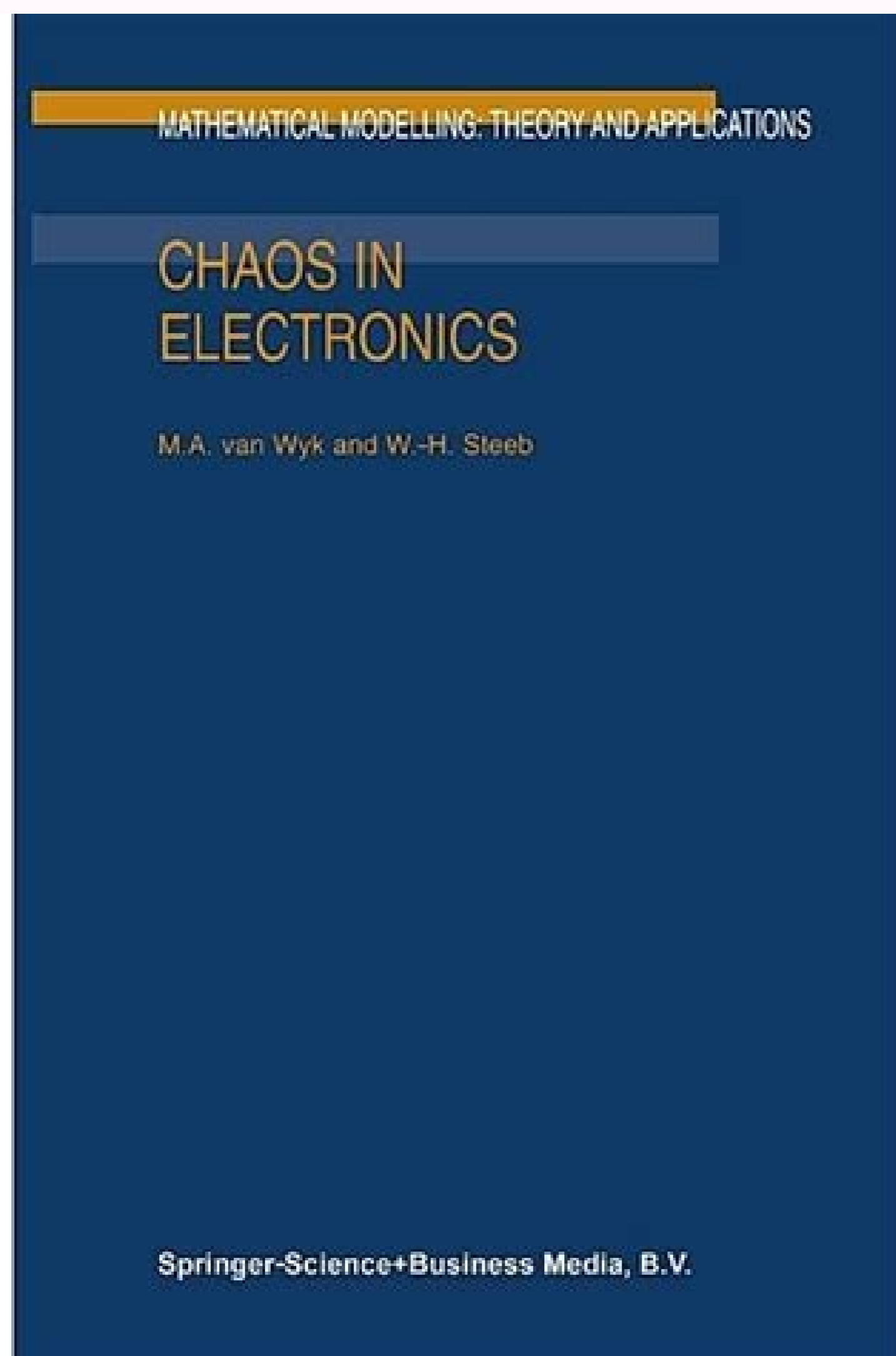
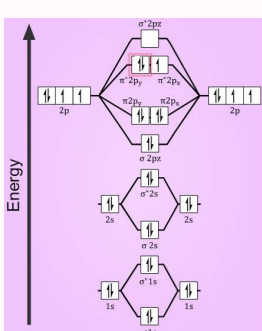




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This is the first complete and up-to-date technical work covering all important aspects of the modern theory of molecular electronic structure. The molecular theory of electronic structure makes extensive use of numerical examples, designed to illustrate the strengths and weaknesses of each method. It is also highly recommended for teaching graduates and advanced graduates. Latest Reviews Latest Reviews "...the most complete and satisfactory presentation of the actual weaponry involved in the computational approach to electronic structure that I have seen, and should be available to all students and researchers who wish to understand the basics of...molecular electronic structure methods." (Physics Today, December 2001) "...the most complete and satisfactory presentation of the actual weaponry involved in the computational approach to electronic structure that I have seen, and should be available to all students and researchers who wish to understand the basics of...methods of molecular electronic structure." (Physics Today, December 2001) "The book offers a deep understanding of basic quantum mechanics..." (Jnl of Solid State Electrochemistry, June 2002) "...the most complete and satisfactory presentation of the actual weaponry involved in the computational approach to electronic structure that I have seen, and should be available to all students and researchers who wish to understand the basics of...methods of molecular electronic structure." (Physics Today, December 2001) "...the book offers a deep understanding of basic quantum mechanics..." (Jnl of Solid State Electrochemistry, June 2002) "...the most complete and satisfactory presentation of the actual weaponry involved in the computational approach to electronic structure that I have seen, and should be available to all students and researchers who understand the basics of...methods of molecular electronic structure." (Physics today, December December The book offers a profound knowledge of basic quantum mechanics..." (Jnl of Solid State Electrochemistry, June 2002) "A the most complete and satisfactory presentation of the actual armament involved in the computational approach to the electronic structure that I have seen and should be available to all students and researchers" (Physics Today, December 2001) Ab initio chimistica  $\hat{A}$  emerged as an important tool in chemical research and  $\hat{A}$  applied to a wide range of problems in chemistry and molecular physics. Quantum chemistry of Ab initio  $\hat{A}$  emerged as an important tool in chemical research and  $\hat{A}$  applied to a wide variety of problems in chemistry and molecular physics. Recent developments in computational methods have enabled previously intractable chemical problems to be solved using rigorous quantum mechanical methods. Topics covered in the book include: Second quantization with spin adaptation Gaussian base set and molecular-integral evaluation Hartree-Fock theory Configuration-interaction and multi-configuration self-coherent theory Coupled-cluster theory for ground and excited states perturbation theory for single and multi-configuration states Linear scale and multi-fast method techniques Explicitly related wavefunctions Convergence of base sets and extrapolation Calibration and benchmarking of computational methods, with applications to molecular equilibrium structures, atomization energies and reaction enthalpies. Poul Jorgensen and Jeppe Olsen Department of Chemistry, University Aarhus, Denmark. Trygve Helgaker, Department of Chemistry, University Oslo, Norway. Problems and exercises are provided at the end of each chapter, complete with suggestions and solutions. This book is a must for researchers in the field of quantum chemistry as well as for non-specialists who acquire an in-depth knowledge of the Ab initio molecular structure theory and its applications for chemistry and physics. In addition, statements about the usefulness and shortcomings of the various methods are supported by real examples, not only by model calculations.

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