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this book represents the proceedings of a symposium held at the spring 1981 acs meeting in atlanta the symposium brought together theoretical chemists solid state physicists experimental chemists and crystallographers one of its major aims was to increase interaction between these diverse groups which often use very different languages to describe similar concepts the development of a common language or at least the acquisition of a multilingual capability is a necessity if the field is to prosper much depends in this field on the interplay between theory and experiment accordingly this volume begins with two introductory chapters one theoretical and the other experimental which contain much of the background material needed for a thorough understanding of the field the remaining sections describe a wide variety of applications and illustrate we believe the central role of charge densities in the understanding of chemical bonding we are most indebted to the divisions of inorganic and physical chemistry of the american chemical society which provided the stimulus for the symposium and gave generous financial support we also gratefully acknowledge financial support from the special educational opportunities program of the petroleum research fund administered by the american chemical society which made extensive participation by speakers from abroad possible

concepts and methods in modern theoretical chemistry electronic structure and reactivity the first book in a two volume set focuses on the structure and reactivity of systems and phenomena a new addition to the series atoms molecules and clusters this book offers chapters written by experts in their fields it enables readers to learn how co

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offering chapters written by experts in their fields this two volume set covers the major areas of research in theoretical chemistry the books enable readers to learn how concepts from ab initio quantum chemistry density functional theory dft and molecular simulation can be used to describe understand and predict electronic structure chemical reactivity and dynamics the first book focuses on the electronic structure and reactivity of many electron systems and the second book deals with the statistical mechanical treatment of collections of such systems

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