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this book explains key concepts in theoretical chemistry and explores practical applications in structural chemistry for experimentalists it highlights concepts that explain the underlying mechanisms of observed phenomena and at the same time provides theoreticians with explanations of the principles and techniques that are important in property design themes covered include conceptual and applied wave functions and density functional theory dft methods electronegativity and hard and soft lewis acid and base hsab concepts hybridization and aromaticity molecular magnetism spin transition and thermochromism offering insights into designing new properties in advanced functional materials it is a valuable resource for undergraduates of physical chemistry cluster chemistry and structure reactivity courses as well as graduates and researchers in the fields of physical chemistry chemical modeling and functional materials

this gentle introduction to high performance computing hpc for data science using the message passing interface mpi standard has been designed as a first course for undergraduates on parallel programming on distributed memory models and requires only basic programming notions divided into two parts the first part covers high performance computing using c with the message passing interface mpi standard followed by a second part providing high performance data analytics on computer clusters in the first part the fundamental notions of blocking versus non blocking point to point communications global communications like broadcast or scatter and collaborative computations reduce with amdalh and gustafson speed up laws are described before addressing parallel sorting and parallel linear algebra on computer clusters the common ring torus and hypercube topologies of clusters are then explained and global communication procedures on these topologies are studied this first part closes with the mapreduce mr model of computation well suited to processing big data using the mpi framework in the second part the book focuses on high performance data analytics flat and hierarchical clustering algorithms are introduced for data exploration along with how to program these algorithms on computer

clusters followed by machine learning classification and an introduction to graph analytics this part closes with a concise introduction to data core sets that let big data problems be amenable to tiny data problems exercises are included at the end of each chapter in order for students to practice the concepts learned and a final section contains an overall exam which allows them to evaluate how well they have assimilated the material covered in the book

includes articles as well as notes and other features about mathematics and the profession

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