Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry)

Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry)

Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry)

The theoretical methods of quantum chemistry have matured to the point that accurate predictions can be made and experiments can be understood for a wide range of important gas-phase phenomena. A large part of this success can be attributed to the maturation of hierarchies of approximation, which allow one to approach very high accuracy, provided that sufficient computational resources are available. Until recently, these hierarchies have not been available in condensed-phase chemistry, but recent advances in the field have now led to a group of methods that are capable of reaching this goal.

Accurate Condensed-Phase Quantum Chemistry addresses these new methods and the problems to which they can be applied. The book begins with an overview of periodic treatments of electron correlation, with an emphasis on the algorithmic features responsible for their computational efficiency. The first section of the book:

- Describes the Laplace-transform approach to periodic second-order perturbation theory (MP2)
- Examines local and density fitted schemes for MP2 in crystalline systems
- Presents test calculations for a variety of systems with small and medium-sized unit cells

The next section focuses on methods based on treatment of the periodic solid in terms of fragments. This part of the book:

- Explores the incremental many-body scheme for electron correlation in solids, and describes progress towards metals and molecules on surfaces
- Describes the hierarchical method as an alternative fragment-based approach to electron correlation in crystalline solids, using conventional molecular electronic structure methods
- Examines electrostatically embedded many-body expansion for large systems, with an emphasis on molecular clusters and molecular liquids
- Explores delocalized and localized orbital approaches to the electronic structures of periodic and non-periodic solids

Lastly, the book describes a practical method by which conventional molecular electronic structure theory can be applied to molecular liquids and solids. Along with the methodology, it presents results on small to medium water clusters as well as on liquid water.

From reader reviews:

Rudy Nixon:

Book is usually written, printed, or outlined for everything. You can know everything you want by a guide. Book has a different type. We all know that that book is important issue to bring us around the world. Beside that you can your reading skill was fluently. A e-book Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry) will make you to become smarter. You can feel considerably more confidence if you can know about everything. But some of you think in which open or reading a book make you bored. It is not make you fun. Why they might be thought like that? Have you seeking best book or suitable book with you?

Cornell Smith:

The actual book Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry) has a lot of information on it. So when you read this book you can get a lot of advantage. The book was compiled by the very famous author. This articles author makes some research prior to write this book. This book very easy to read you can find the point easily after reading this book.

Roxie Lloyd:

Exactly why? Because this Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry) is an unordinary book that the inside of the book waiting for you to snap the idea but latter it will shock you with the secret it inside. Reading this book close to it was fantastic author who write the book in such amazing way makes the content on the inside easier to understand, entertaining technique but still convey the meaning thoroughly. So , it is good for you because of not hesitating having this any longer or you going to regret it. This excellent book will give you a lot of positive aspects than the other book have such as help improving your talent and your critical thinking method. So , still want to postpone having that book? If I had been you I will go to the publication store hurriedly.

Roman Morris:

Reading a guide make you to get more knowledge from it. You can take knowledge and information from a book. Book is composed or printed or highlighted from each source that filled update of news. With this modern era like right now, many ways to get information are available for anyone. From media social like newspaper, magazines, science publication, encyclopedia, reference book, novel and comic. You can add your understanding by that book. Are you hip to spend your spare time to spread out your book? Or just seeking the Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry) when you required it?

Download and Read Online Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry) #JGLCNKD9WM2

Read Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry) for online ebook

Online Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry) ebook PDF download

Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry) Doc

Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry) Mobipocket

Accurate Condensed-Phase Quantum Chemistry (Computation in Chemistry) EPub