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Physical Chemistry

A Molecular Approach

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Physical Chemistry A Molecular Approach

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taught by bridging the gap between the traditional solve a bunch of equations for a very simple model approach and the computational methods that are used to solve research problems This book will revolutionize the way physical chemistry is taught by bridging the gap between the traditional solve a bunch of equations for a very simple model approach and the computational methods that are used to solve research problems While some recent textbooks include exercises using pre packaged Hartree Fock DFT calculations this is largely limited to giving students a proverbial black box The DIY do it yourself approach taken in this book helps student gain understanding by building their own simulations from scratch The reader of this book should come away with the ability to apply and adapt these techniques in computational chemistry to his or her own research problems and have an enhanced ability to critically evaluate other computational results This book is mainly intended to be used in conjunction with an existing physical chemistry text such as McQuarrie Simon s Physical Chemistry A Molecular Approach but it is also well suited as a stand alone text for upper level undergraduate or intro graduate computational chemistry courses Assumes no computational background Enables students to build simulations from scratch to reproduce famous literature calculations Teaches a variety of computational numerical simulation methods applicable to solving chemical problems Designed to play well with McQuarrie Simon s landmark P CHEM text but can be used with others as well

Basic Physical Chemistry E Brian Smith,2012-06-26 This elegant book provides a student friendly introduction to the subject of physical chemistry It is concise and more compact than standard textbooks on the subject and it emphasises the two important concepts underpinning physical chemistry quantum mechanics and the second law of thermodynamics The principles are challenging to students because they both focus on uncertainty and probability The book explains these fundamental concepts clearly and shows how they offer the key to understanding the wide range of chemical phenomena including atomic and molecular spectra the structure and properties of solids liquids and gases chemical equilibrium and the rates of chemical reactions

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followed by a practice exercise Molecular Physical Chemistry José J. C. Teixeira-Dias,2017-01-16 This is the physical chemistry textbook for students with an affinity for computers It offers basic and advanced knowledge for students in the second year of chemistry masters studies and beyond In seven chapters the book presents thermodynamics chemical kinetics quantum mechanics and molecular structure including an introduction to quantum chemical calculations molecular symmetry and crystals The application of physical chemical knowledge and problem solving is demonstrated in a chapter on water treating both the water molecule as well as water in condensed phases Instead of a traditional textbook top down approach this book presents the subjects on the basis of examples exploring and running computer programs Mathematica discussing the results of molecular orbital calculations performed using Gaussian on small molecules and turning to suitable reference works to obtain thermodynamic data Selected Mathematica codes are explained at the end of each chapter and cross referenced with the text enabling students to plot functions solve equations fit data normalize probability functions manipulate matrices and test physical models In addition the book presents clear and step by step explanations and provides detailed and complete answers to all exercises In this way it creates an active learning environment that can prepare students for pursuing their own research projects further down the road Students who are not yet familiar with Mathematica or Gaussian will find a valuable introduction to computer based problem solving in the molecular sciences Other computer applications can alternatively be used For every chapter learning goals are clearly listed in the beginning so that readers can easily spot the highlights and a glossary in the end of the chapter offers a quick look up of important terms *Physical Chemistry for the Chemical Sciences* Raymond Chang,2014-06-15 Following in the wake of Chang s two other best selling physical chemistry textbooks *Physical Chemistry for the Chemical and Biological Sciences* and *Physical Chemistry for the Biosciences* this new title introduces laser spectroscopist Jay Thoman Williams College as co author Following in the wake of Chang s two other best selling physical chemistry textbooks *Physical Chemistry for the Chemical and Biological Sciences* and *Physical Chemistry for the Biosciences* this new title introduces laser spectroscopist Jay Thoman Williams College as co author This comprehensive new text has been extensively revised both in level and scope Targeted to a mainstream physical chemistry course this text features extensively revised chapters on quantum mechanics and spectroscopy many new chapter ending problems and updated references while biological topics have been largely relegated to the previous two textbooks Other topics added include the law of corresponding states the Joule Thomson effect the meaning of entropy multiple equilibria and coupled reactions and chemiluminescence and bioluminescence One way to gauge the level of this new text is that students who have used it will be well prepared for their GRE exams in the subject Careful pedagogy and clear writing throughout combine to make this an excellent choice for your physical chemistry course **Molecular Approach of Modern Physical Chemistry** Ved Prakash Patial,2016 **Physical Chemistry** Peter Atkins,Julio de Paula,Ronald Friedman,2014 This title takes an innovative molecular approach to the teaching of physical chemistry The authors present

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