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**Applied Theoretical Organic Chemistry** Tantillo Dean J,2018-03-07 This book provides state-of-the-art information on how studies in applied theoretical organic chemistry are conducted. It highlights the many approaches and tools available to those interested in using computational chemistry to predict and rationalize structures and reactivity of organic molecules. Chapters not only describe theoretical techniques in detail, but also describe recent applications and offer practical advice. Authored by many of the world leaders in the field of applied theoretical chemistry, this book is perfect for both practitioners of computational chemistry and synthetic and mechanistic organic chemists curious about applying computational techniques to their research. Contents: Modeling Organic Reactions — General Approaches, Caveats, and Concerns (Stephanie R Hare, Brandi M Hudson and Dean J Tantillo)Overview of Computational Methods for Organic Chemists (Edyta M Greer and Kitae Kwon)Brief History of Applied Theoretical Organic Chemistry (Steven M Bachrach)Solvation (Carlos Silva Lopez and Olalla Nieto Faza)Conformational Searching for Complex, Flexible Molecules (Alexander C Brueckner, O Maduka Ogba, Kevin M Snyder, H Camille Richardson and Paul Ha-Yeon Cheong)NMR Prediction (Kelvin E Jackson and Robert S Paton)Energy Decomposition Analysis and Related Methods (Israel Fernández)Systems with Extensive Delocalization (L Zoppi and K K Baldrige)Modern Treatments of Aromaticity (Judy I-Chia Wu)Weak Intermolecular Interactions (Rajat Maji and Steven E Wheeler)Predicting Reaction Pathways from Reactants (Romain Ramozzi, W M C Sameera and Keiji Morokuma)Unusual Potential Energy Surfaces and Nonstatistical Dynamic Effects (Charles Doubleday)The Distortion/Interaction Model for Analysis of Activation Energies of Organic Reactions (K N Houk, Fang Liu, Yun-Fang Yang and Xin Hong)Spreadsheet-Based Computational Predictions of Isotope Effects (O Maduka Ogba, John D Thoburn and Daniel J O'Leary)Stereoelectronic Effects: Analysis by Computational and Theoretical Methods (Gabriel dos Passos Gomes and Igor Alabugin)pKa Prediction (Yijie Niu and Jeehiun K Lee)Issues Particular to Organometallic Reactions (Gang Lu, Huiling Shao, Humair Omer and Peng Liu)Computationally Modeling Nonadiabatic Dynamics and Surface Crossings in Organic Photoreactions (Arthur Winter)Challenges in Predicting Stereoselectivity (Elizabeth H Krenske) Readership: Practitioners of computational chemistry and synthetic and mechanistic organic chemists curious about applying computational techniques to their research. Keywords: Organic Chemistry;Theoretical Chemistry;Stereoselectivity;NMR Prediction;pKa Prediction;Organic PhotoreactionsReview: Key Features: A particular strength is the mix of theoretical background, informative examples and practical advice providedChapters are authored by many of world leaders in the field of applied theoretical chemistry

**Fundamentals of Time-Dependent Density Functional Theory** Miguel A.L. Marques,Neepa T. Maitra,Fernando M.S. Nogueira,E.K.U. Gross,Angel Rubio,2012-01-20 There have been many significant advances in time-dependent density functional theory over recent years, both in enlightening the fundamental theoretical basis of the theory, as well as in computational algorithms and applications. This book, as successor to the highly successful volume Time-Dependent Density Functional Theory (Lect. Notes Phys. 706, 2006) brings together for the first time all recent developments in a systematic and coherent way. First, a thorough pedagogical presentation of the fundamental theory is given, clarifying aspects of the original proofs and theorems, as well as presenting fresh developments that extend the theory into new realms—such as alternative proofs of the original Runge-Gross theorem, open quantum systems, and dispersion forces to name but a few. Next, all of the basic concepts are introduced sequentially and building in complexity, eventually reaching the level of open problems of interest. Contemporary applications of the theory are discussed, from real-time coupled-electron-ion dynamics, to excited-state dynamics and molecular transport. Last but not least, the authors introduce and review recent advances in computational implementation, including massively parallel architectures and graphical processing units. Special care has been taken in editing this volume as a multi-author textbook, following a coherent line of thought, and making all the relevant connections between chapters and concepts consistent throughout. As such it will prove to be the text of reference in this field, both for beginners as well as expert researchers and lecturers teaching advanced quantum mechanical methods to model complex physical systems, from molecules to nanostructures, from biocomplexes to surfaces, solids and liquids. From the reviews of LNP 706: “This is a well structured text, with a common set of notations and a single comprehensive and up-to-date list of references, rather than just a compilation of research articles. Because of its clear organization, the book can be used by novices (basic knowledge of ground-state DFT is assumed) and experienced users of TD-DFT, as well as developers in the field.” (Anna I. Krylov, Journal of the American Chemical Society, Vol. 129 (21), 2007) “This book is a treasure of knowledge and I highly recommend it. Although it is a compilation of chapters written by many different leading researchers involved in development and application of TDDFT, the contributors have taken great care to make sure the book is pedagogically sound and the chapters complement each other [...]. It is highly accessible to any graduate student of chemistry or physics with a solid grounding in many-particle quantum mechanics, wishing to understand both the fundamental theory as well as the exponentially growing number of applications. [...] In any case, no matter what your background is, it is a must-read and an excellent reference to have on your shelf.” Amazon.com, October 15, 2008, David Tempel (Cambridge, MA)

**Congressional Record** United States. Congress,2011 The Congressional Record is the official record of the proceedings and debates of the United States Congress. It is published daily when Congress is in session. The Congressional Record began publication in 1873. Debates for sessions prior to 1873 are recorded in The Debates and Proceedings in the Congress of the United States (1789-1824), the Register of Debates in Congress

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Gold Chemistry Mohr,2009-03-12 Written by world-class authors, this most recent major book on the topic highlights new and current trends as well as future directions. It is comprehensive in its scope, covering all aspects of gold chemistry -- from homogeneous to heterogeneous catalysis, from supramolecular assemblies to sensors and medicinal applications. The result is an invaluable work for both organic and inorganic chemists working in universities and industry, as well as material scientists.

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