Book Review: *Exploring Chemistry with Electronic Structure Methods*, Second edition, James B. Foresman and AEleen Frisch. Published by Gaussian, Inc., Pittsburgh, PA, 15106 USA. 354 pages. Soft cover: $42.00 ISBN 0-9636769-3-8, Hard cover: $100.00 ISBN 0-9636769-4-6

Abraham F. Jalbout [1,2,3]

[1] *Department of Physics, Dillard University, New Orleans, LA 70112*
[2] *Department of Chemistry, The University of New Orleans, New Orleans, LA 70148*
[3] *EJMAPS Organization, 1107 Carrollton Ave, Metairie, LA 70005*

Received 27-11-2002

In this book an attempt has been made to introduce readers how the electronic structure modeling can be use to investigate about different chemical phenomena. The Gaussian package gives the ability for Prediction of many molecular properties such as, molecular structure and energies, energy and structure of transition states, reaction pathways, (IR, NMR,…) properties, atomic charge and electrostatic potentials, multipole moments, polarizabilities and hyperpolarizabilities,… in gas phase or in solution.

Exploring Chemistry with Electronic Structure Methods is a work that structured as a study guide for chemist to learn how employs different keyword of Gaussian package to obtain the above properties.

This book begins with a *(Gaussian Quick Start)* Tutorial designed to help new Gaussian users begin using the program right away. The remainder of the work is divided into three main parts. In the first part *(Essential Concepts and Techniques)* computational chemistry and the principal sorts of predictions which can be made using electronic structure theory is introduced. *(Model Chemistries)* is the second part that provides an in-depth examination of the accuracy, scope of applicability and other characteristics and trade-offs of all of the major well-defined electronic structure models. It also gives some general recommendations for selecting the best model for investigating a particular problem.

(Applications) is the third part that contains discussion about electronic structure calculations in the context of real-life research situations, focusing on how it can be used to illuminate a variety of chemical problems.

In this book each chapter focuses on a single topic, and includes explanations of the chemical phenomena under consideration and the relevant computational properties, one or two detailed examples of setting up such calculations and interpreting their results. Several exercises designed to both provide practice on the area and to introduces its more advanced aspects.

Experimental research chemist, students of physical chemistry and experienced gaussian users will benefit from reading this book.