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Preface

Annual Reports in Computational Chemistry (ARCC) provides reviews and/or highlighted summaries of research areas relevant to the broad field of computational chemistry. This field continues to evolve from its early beginnings into a critical component of the current toolbox in use by chemists. This evolution is proceeding at a more rapid pace due to continued improvements in theory and algorithm developments, software implementations, and hardware, with the latter driven by advances in the entertainment/gaming industry. A goal of the series is to provide reviews not only for experts in the field but also for students who are interested in learning how to use computational methods to address real problems in chemistry. For this reason, the authors provide complete references as well as more details than are often provided in the literature. Volume 16 continues to expand on these concepts with five chapters, which are focused on a range of exciting new computational chemistry developments. These chapters range from basic quantum mechanics, to the treatment of relativistic effects, to the quantum treatment of nuclear motion, to the role of solvent dynamics, and finally to how quantum chemistry can be used to explain reactions in the Earth’s atmosphere.

This volume has a focus on some of the basic theoretical concepts underlying modern quantum chemistry. Chapter 1 by Smith presents a formulation of quantum mechanics based on quantization of Hamilton’s equations of classical dynamics coupled with the classical phase space density. Smith shows that the Schrödinger equation is readily derived in this approach and that the approach is consistent with the Heisenberg approach as well. He presents an application of this new formulation to the harmonic oscillator, obtaining an analytical solution. He shows how the dynamics in this approach can be used to construct the quantum time correlation function.

Relativistic quantum chemistry is allowing chemists to delve more deeply into the electronic structure of heavy elements for which experimental data is often lacking due to the difficulty in making the atoms so that they are very scarce and to their radioactivity. Chapter 2 by Zhang, Kasper, and Li provides a description of localized two-component approximations to the solution of the Dirac equation so that chemists can study relativistic effects in larger molecular systems with higher accuracy by reducing the computational cost. They introduce a maximally localized variant, the atomically
localized Hamiltonian, which can be used for molecular or periodic systems. They describe the implementation of the approach in the open-source Chronus Quantum package. They use their approaches to predict the excited states of Pt$_2$ and the L$_{2,3}$-edge X-ray absorption spectra of transition metal complexes.

In Chapter 3, Garashchuk and Rassolov move from quantum effects in electronic motion to the development of methods for the treatment of quantum effects for nuclear motion in molecular dynamics simulations. They base their developments on the quantum trajectory, (Bohmian) formulation of the time-dependent Schrödinger equation. They employ the approximation of the Linearized Quantum Force as it is stable and exhibits linear scaling with the system size. The methods they describe can be applied to dynamically active quantum subsystems, especially those that involve diffusion and thermal processes coupled to the molecular environment, which help to overcome the inherent temporal instability of Bohmian dynamics.

The time-dependent Stokes shift allows one to probe solvation dynamics which may influence a chemical reaction beyond the mean field effects which are modeled by a self-consistent reaction field approach. In Chapter 4, Schröder and Heid describe how the time-dependent Stokes shift can be modeled and how the simulations can be used to obtain a detailed analysis of the underlying molecular processes, including the roles of different solvent shells. They show the importance of using polarizable force fields in their simulations based on classical molecular dynamics. The results allowed the authors to determine the role of solvent motion vs chromophore motion as well as the number of replicas needed for equilibrium vs nonequilibrium dynamics. They present applications to the prediction of the properties of neutral and ionic liquids, hydration dynamics near micelles and reverse micelles, and solvation dynamics close to biomolecules including proteins and DNA.

The final Chapter 5 by Zhong and Francisco describes the application of a variety of high level electronic structure methods to atmospheric chemistry. Although many of the chemical processes in the atmosphere are governed by simple bimolecular reactions, it has become increasingly evident over the past decade that many atmospheric processes are governed by more complex processes, including catalytic ones. The authors first describe homogeneous catalytic reactions including SO$_3$ with H$_2$O, H$_2$S, and CH$_3$OH showing the importance of proton donor/acceptor capabilities, and hydrolysis of and the reactions of amines with formaldehyde. They then describe selected autocatalytic and heterolytic catalyzed reactions, with the latter having a focus again on the reactions of SO$_3$. 
This book was put together in a difficult year due to the COVID-19 pandemic and I am extremely grateful to the contributions from the authors during this time. This effort would also not have been successful without the efforts of Leticia Lima from Elsevier to keep this series going and helping me to develop a useful and quality volume in this series. We hope that you will find this series useful and interesting. We are currently working on Volume 17 and welcome contributions to it and subsequent volumes. We will continue to expand the sections to include even more branches of computational chemistry. Do not hesitate to contact the Editor with suggestions of topics to be covered or to volunteer providing a chapter.

Dr. David A. Dixon, Editor
Robert Ramsay Chair
The University of Alabama