JCTC Journal of Chemical Theory and Computation

Editorial

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Developments in Theoretical Chemistry

The development and characterization of theoretical approaches has become an increasingly indispensable area of physical chemistry since its earliest days. The advent of quantum mechanics, more than a century ago, and the exponential growth of computational resources have changed the way we look at theoretical and computational approaches to research. Today, the majority of manuscripts submitted to *The Journal of Physical Chemistry* (*JPC*) contain some computational aspect to the research that is discussed. This trend is not new, however, and was recognized nine years ago when, in recognition of the importance of theory and computation in the chemical research endeavor, ACS launched a journal solely dedicated to this work, the *Journal of Chemical Theory and Computation* (*JCTC*).

In the compilation of papers that are assembled in this Virtual Issue, *The Journal of Physical Chemistry A* (*JPC A*) and *JCTC* have joined together to highlight recently published manuscripts that have made an appreciable impact on the modern developments in theory and computation. These two journals provide complementary venues for such work.

The selection of papers from *JPC A* illustrates the range of approaches that are being pursued to extend the reach of dynamics calculations. Many of these papers provide theoretical and computational methodologies for studying related problems in kinetics, dynamics, spectroscopy, and excited states which are then applied to the core areas of experimentally focused work that is published in *JPC A*, including astrochemsitry, atmospheric chemistry, etc. For example, the contribution by Georgievskii et al. provides a new formulation of the master equation for chemical reactions involving multiple isomers and intermediates, providing expressions that can be used to obtain the phenomenological rate coefficients for such processes. Likewise, Kishi and Nakano developed a quantum master equation to evaluate dynamic polarizabilities, which can be used, for example, to evaluate static and dynamic response properties of radicals in a nonperturbative manner. In the contribution of Evangelista et al., the authors describe a time-independent DFT approach for evaluating excitation energies, applying it to a range of organic molecules. As is characteristic of *JPC A*, the theoretical contributions focus on the development of theoretical and computational approaches that can be used to study and gain insights into complementary experimentally measured phenomena.

The selection of papers from *JCTC* reflects the central role that density functional theory currently plays in computational quantum chemistry. Development of novel and more accurate functionals continues unabated, although perhaps unfortunately, a good dose of empiricism has in many instances replaced first-principles construction. The current selection of *JCTC* papers for this Virtual Issue includes manuscripts on double hybrids (Goerigk and Grimme), meta and hybrid-meta functionals (Zhao and Truhlar), and excitation energies with range-separated exchange−correlation kernels (Kronik et al.). Benchmarking of functionals over extensive databases has also become an important topic in DFT. Also included is a paper by Rezac et al., where the S-66 database is presented. Steinmann and Corminboeuf benchmark density-dependent dispersion corrections. In the past few years, *JCTC* has published many research articles on DFT that have become milestones in this field, and the sample presented here is only a small token of a much larger body of work.

Through this compilation, listed in Table 1, we hope to provide an overview of some of the interesting and exciting theoretical and computational development work recently published in *JPC A* and *JCTC*.

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Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

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Table 1. Selected Recent Theoretical Chemistry Papers From *The Journal of Physical Chemistry A* and *Journal of Chemical Theory and Computation* Included in This Collection

reference number	title	authors	citation
1	Remarks on the Validity of the Fixed Nuclei Approximation in Quantum Electron Dynamics	Inga S. Ulusoy and Mathias Nest	*J. Phys. Chem. A* **2012**, *116* (46), 11107−11110. DOI: 10.1021/jp304140r
2	Numerical Implementation and Test of the Modified Variational Multiconfigurational Gaussian Method for High-Dimensional Quantum Dynamics	Miklos Ronto and Dmitrii V. Shalashilin	*J. Phys. Chem. A* **2013**, *117* (32), 6948−6959. DOI: 10.1021/jp310976d
3	Symmetrical Windowing for Quantum States in Quasi-Classical Trajectory Simulations	Stephen J. Cotton and William H. Miller	*J. Phys. Chem. A* **2013**, *117* (32), 7190−7194. DOI: 10.1021/jp401078u
4	Orthogonality Constrained Density Functional Theory for Electronic Excited States	Francesco A. Evangelista, Philip Shushkov, and John C. Tully	*J. Phys. Chem. A* **2013**, *117* (32), 7378−7392. DOI: 10.1021/jp401323d
5	Langevin Equation Path Integral Ground State	Steve Constable, Matthew Schmidt, Christopher Ing, Tao Zeng, and Pierre-Nicholas Roy	*J. Phys. Chem. A* **2013**, *117* (32), 7461−7467. DOI: 10.1021/jp4015178
6	Quasi-Classical Theory of Electronic Flux Density in Electronically Adiabatic Molecular Processes	D. J. Diestler	*J. Phys. Chem. A* **2012**, *116* (46), 11161−11166. DOI: 10.1021/jp304747a
7	Reformulation and Solution of the Master Equation for Multiple-Well Chemical Reactions	Yuri Georgievskii, James A. Miller, Michael P. Burke, and Stephen J. Klippenstein	*J. Phys. Chem. A* **2013**, *117* (46), 12146−12154. DOI: 10.1021/jp4060704
8	Time-Resolved Femtosecond Photoelectron Spectroscopy by Field-Induced Surface Hopping	Roland Mitrić, Jens Petersen, Matthias Wohlgemuth, Ute Werner, Vlasta Bonačić-Koutecký, Ludger Wöste, and Joshua Jortner	*J. Phys. Chem. A* **2011**, *115* (16), 3755−3765. DOI: 10.1021/jp106355n
9	Open Quantum System Approach to the Modeling of Spin Recombination Reactions	M. Tiersch, U. E. Steiner, S. Popescu, and H. J. Briegel	*J. Phys. Chem. A* **2012**, *116* (16), 4020−4028. DOI: 10.1021/jp209196a
10	Quantum Master Equation Method Based on the Broken-Symmetry Time-Dependent Density Functional Theory: Application to Dynamic Polarizability of Open-Shell Molecular Systems	Ryohei Kishi and Masayoshi Nakano	*J. Phys. Chem. A* **2011**, *115* (15), 3565−3575. DOI: 10.1021/jp200056m
11	Efficient and Accurate Double-Hybrid-Meta-GGA Density Functionals—Evaluation with the Extended GMTKN30 Database for General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions	Lars Goerigk and Stefan Grimme	*J. Chem. Theory Comput.* **2011**, *7* (2), 291−309. DOI: 10.1021/ct100466k
12	S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures	Jan Řezáč, Kevin E. Riley, and Pavel Hobza	*J. Chem. Theory Comput.* **2011**, *7* (8), 2427−2438. DOI: 10.1021/ct2002946
13	Assessment of the Performance of DFT and DFT-D Methods for Describing Distance Dependence of Hydrogen-Bonded Interactions	Kanchana S. Thanthiriwatte, Edward G. Hohenstein, Lori A. Burns, and C. David Sherrill	*J. Chem. Theory Comput.* **2011**, *7* (1), 88−96. DOI: 10.1021/ct100469b
14	Density Functional Theory for Reaction Energies: Test of Meta and Hybrid Meta Functionals, Range-Separated Functionals, and Other High-Performance Functionals	Yan Zhao and Donald G. Truhlar	*J. Chem. Theory Comput.* **2011**, *7* (3), 669−676. DOI: 10.1021/ct1006604
15	Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals	Leeor Kronik, Tamar Stein, Sivan Refaely-Abramson, and Roi Baer	*J. Chem. Theory Comput.* **2012**, *8* (5), 1515−1531. DOI: 10.1021/ct2009363
16	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals	Noa Marom, Alexandre Tkatchenko, Mariana Rossi, Vivekanand V. Gobre, Oded Hod, Matthias Scheffler, and Leeor Kronik	*J. Chem. Theory Comput.* **2011**, *7* (12), 3944−3951. DOI: 10.1021/ct2005616
17	Time-Dependent Density-Functional Description of the ^1L_a State in Polycyclic Aromatic Hydrocarbons: Charge-Transfer Character in Disguise?	Ryan M. Richard and John M. Herbert	*J. Chem. Theory Comput.* **2011**, *7* (5), 1296−1306. DOI: 10.1021/ct100607w
18	A Qualitative Index of Spatial Extent in Charge-Transfer Excitations	Tangui Le Bahers, Carlo Adamo, and Ilaria Ciofini	*J. Chem. Theory Comput.* **2011**, *7* (8), 2498−2506. DOI: 10.1021/ct200308m
19	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction	Stephan N. Steinmann and Clemence Corminboeuf	*J. Chem. Theory Comput.* **2011**, *7* (11), 3567−3577. DOI: 10.1021/ct200602x
20	First Principles Simulations of the Infrared Spectrum of Liquid Water Using Hybrid Density Functionals	Cui Zhang, Davide Donadio, François Gygi, and Giulia Galli	*J. Chem. Theory Comput.* **2011**, *7* (5), 1443−1449. DOI: 10.1021/ct2000952
21	Assessing Excited State Methods by Adiabatic Excitation Energies	Robert Send, Michael Kühn, and Filipp Furche	*J. Chem. Theory Comput.* **2011**, *7* (8), 2376−2386. DOI: 10.1021/ct200272b
22	Evaluating the Performance of DFT Functionals in Assessing the Interaction Energy and Ground-State Charge Transfer of Donor/Acceptor Complexes: Tetrathiafulvalene−Tetracyanoquinodimethane (TTF−TCNQ) as a Model Case	Gjergji Sini, John S. Sears, and Jean-Luc Brédas	*J. Chem. Theory Comput.* **2011**, *7* (3), 602−609. DOI: 10.1021/ct1005517