

# MQM 2022: The 10th Triennial Conference on Molecular Quantum Mechanics

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We are pleased to introduce this virtual special issue (VSI) of the *Journal of Physical Chemistry* containing the proceedings of the 10th Molecular Quantum Mechanics conference. MQM 2022 follows a long and distinguished tradition of conferences dedicated to honoring the achievements of leading scientists in the field and highlighting the superb science of the international quantum chemistry community. The MQM series of conferences was founded by Nicholas C. Handy and Henry F. (Fritz) Schaefer III, who hosted the first meeting at the University of Georgia in 1989 in honor of John Pople (who would go on to win the Nobel Prize in Chemistry in 1998). In 1995, the second conference was held at the University of Cambridge in memory of Samuel Francis Boys and in honor of Isaiah Shavitt, followed by MQM 2001 at the University of Washington honoring Ernest Davidson. Subsequent to the meeting in Seattle, MQM shifted to a triennial schedule with the next conferences held once again in Cambridge in honor of Nicholas Handy (2004); Budapest in honor of Peter Pulay (2007); Berkeley in honor of Fritz Schaefer (2010); Lugano, Switzerland, in honor of Rodney Bartlett (2013); Uppsala, Sweden, in memory of Jan Almlöf, Inga Fischer-Hjalmars, Per-Olov Löwdin, and Bjorn Roos and in honor of Per Siegbahn (2016); and finally in Heidelberg, Germany, in memory of Reinhart Ahlrichs and in honor of Werner Kutzelnigg, Wilfried Meyer, and Sigrid Peyerimhoff (2019).

MQM 2022 was held at Virginia Tech in Blacksburg, Virginia, June 26th through July first, 2022, in honor of Martin Head-Gordon and Gustavo Scuseria, both of whom have made — and continue to make — long-lasting contributions to the field of quantum chemistry, particularly in the development of new methods and algorithms. The conference was organized by the authors of this Preface and was one of the first major international meetings in the field to be held fully in person in the waning months of the COVID-19 pandemic. More than 200 scientists from 11 different countries participated in the meeting, giving more than 50 lectures and over 130 poster presentations. Four historical lectures were given to recognize the many accomplishments of the two honorees by Profs. Peter M. W. Gill (University of Sydney), Fritz Schaefer (University of Georgia), Krishnan Raghavachari (Indiana University), and C. David Sherrill (Georgia Tech).

This VSI collects 34 manuscripts reporting original new research that was associated with MQM 2022. While most of these appeared in *J. Phys. Chem. A* — particularly section A4:

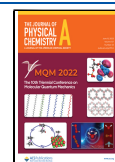
New Tools and Methods in Experiment and Theory — a few were published in parts B and C of the *Journal*, which is indicative of the ever-expanding scope of MQM.

## NEW QUANTUM MECHANICAL METHODS AND TOOLS

The MQM series of conferences is well-known for highlighting emerging quantum chemical methods, and MQM 2022 was no exception. In the only Review Article in this VSI, Harsha at the University of Michigan along with Henderson and Scuseria at Rice University give an overview of recent developments in thermofield theory and finite-temperature electronic structure methods.<sup>1</sup> Along with a detailed reprise of the underlying theory, they provide a series of benchmark examples using the one-dimensional Hubbard model and a preview of coming developments in this area. Vu and co-workers in the DePrince group at Florida State University have developed a quantum electrodynamics extension to time-dependent density functional theory (TD-DFT).<sup>2</sup> They apply the new method to the chiral group-directed photoisomerization of the BINOL molecule and demonstrate that strong light-matter coupling can alter its diastereomeric excess. In other work, Wang of Sophysics Technology in collaboration with Li and Zhang of the University of Florida test self-consistent effective Hamiltonian theory by applying it to an Anderson-Hubbard Hamiltonian.<sup>3</sup> They find that the numerical solution to a model problem yields the correct Kondo resonance in the quasi-particle density of states.

In the DFT domain, Perdew and co-workers report on the usefulness of the strongly constrained and appropriately normed (SCAN) meta-generalized gradient approximation (meta-GGA) density functional in describing strong electron-correlation effects.<sup>4</sup> Using singlet C<sub>2</sub> as a test case, they find that spin symmetry breaking corrects artifactual underbinding that yields a reduced atomization energy for that difficult molecule. Roy, Cuierrier, and Ernzerhof at Université de Montréal propose a simplification of various approaches to the

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use of correlation factors for modeling exchange-correlation holes in DFT.<sup>5</sup> Their approach allows for self-consistent implementations of such functionals, which they test using a new meta-GGA. Oueis, Sizov, and Staroverov at the University of Western Ontario report an extension of their previous work on representations of exchange-correlation potentials within a set of linearly independent products.<sup>6</sup> They find that extending the underlying one-electron basis set to include low-lying virtual orbitals significantly improves the representation of the original potential. Finally, a reformulation of a combined DFT/multireference configuration interaction (MRCI) approach is reported by Dombrowski and co-workers in the Marian group at the Heinrich-Heine-Universität Düsseldorf involving a new effective Hamiltonian using a splitting of parameters associated with intra- and interorbital interactions.<sup>7</sup> Based on their statistical analysis of the performance of this new method, they recommend it be considered the new standard for such calculations.

Focusing on wave function-based models, Kulahlioglu and Dreuw at Universität Heidelberg report the development of a multistate formulation of the quantum Monte Carlo algebraic diagrammatic construction that allows for massively parallel implementations.<sup>8</sup> They find that the new method can reproduce the excitation energies of multiple low-lying states with controllable errors. Savin and Karwowski at the Sorbonne Université and Nicolaus Copernicus University, respectively, examined the sources of error arising from the use of long-range approximations to the Coulomb potential.<sup>9</sup> They report that such errors may be reduced by including generalized cusp conditions in the wave function representation for small electron–electron distances. Finally, in the only MQM VSI contribution appearing in the *Journal of Physical Chemistry B*, Hirata of the University of Illinois, Shigeta of University of Tsukuba, Xantheas of Pacific Northwest National Laboratory, and Bartlett of the Quantum Theory Project at the University of Florida introduce an *ab initio* second-order many-body Green's function method for infinite helical polymers.<sup>10</sup> Their approach allows for the calculation of a wide range of properties of such species, and they apply it to a set of paradigmatic polymers for which they compute structures, infrared and Raman frequencies, phonon dispersions, and inelastic neutron scattering spectra.

## ■ WEAK INTERACTIONS, SOLVATION, AND DECOMPOSITION METHODS

A long-standing challenge in quantum chemistry is the description and understanding of weak interactions, including those between solvent and solute. Anstötter and co-workers from the Matsika group at Temple University examined the performance of the effective fragment potential (EFP) method in the description of electronically excited states in micro-solvated systems.<sup>11</sup> In particular, they used equation-of-motion coupled cluster (EOM-CC) to calculate vertical excitation energies and vertical attachment energies of solvated indole with both EFP and fully quantum mechanical solvent, finding minimal differences between the approaches. Next, in an effort to avoid the system-size limitations and inaccuracies of many models of explicit solvation, Rahbar and Stein propose a statistical thermodynamic model based on the grand canonical ensemble framework.<sup>12</sup> They test their generalized approach using a Lennard-Jones model fluid.

Equally important to simulating weak interactions is the question of how to decompose them into fundamental components. Aldossary and co-workers from the T. Head-

Gordon and M. Head-Gordon groups at Berkeley describe a new method to decompose intermolecular forces into typical components of electrostatic, Pauli repulsion, van der Waals, and charge-transfer contributions.<sup>13</sup> They test the method using systems such as the water dimer and a water molecule interacting with sodium chloride and find that it serves as a useful complement to the well-known energy decomposition analysis. In somewhat related work, Luu and Patkowski at Auburn University report on their improvements to the intramolecular symmetry-adapted perturbation theory (ISAPT) method for decomposing the noncovalent interaction energy between two molecular fragments connected by a linker.<sup>14</sup> They make use of new partitioning algorithms to overcome problems with electrostatic, induction, and exchange-induction components. Next, in an effort to understand the nature of  $\pi$ -stacking in porous, conjugated aromatic frameworks, Gray and Herbert at The Ohio State University used extended SAPT to decompose the interaction energies of several representative systems, including the [18]annulene dimer.<sup>15</sup> In their paper, which appears in section C4 (“Physical Properties of Materials and Interfaces”) of *J. Phys. Chem. C*, they found that van der Waals interactions drive the structural preferences of these frameworks, which adopt a slip-stacked geometry.

## ■ NEW ALGORITHMS IN QUANTUM CHEMISTRY

As quantum chemical methods improve, so, too, must efficient implementations thereof. In an effort to streamline the calculation of two-electron repulsion integrals (ERIs) in quantum chemical calculations, Black and co-workers in the Gill group at the University of Sydney report on an effort to identify and screen insignificant shell-pairs and -quartets in the evaluation of such integrals over Gaussian basis functions.<sup>16</sup> In their numerical tests using a fragment extracted from a protein, they found that the Hölder inequality is preferable for pairs and the Cauchy-Schwarz inequality is preferable for quartets. Heat-bath configuration interaction (HCI) methods are the focus of a paper by the Zimmerman group at the University of Michigan,<sup>17</sup> and they report on a series of algorithmic improvements that take advantage of distributed- and shared-memory parallelism to achieve highly scalable performance. Next, Melo, Pederson, and Peralta describe an implementation of the Fermi-Löwdin orbital self-interaction correction (FLOSIC) method that is suitable for existing quantum chemistry programs.<sup>18</sup> They examine the convergence behavior of the algorithm for properties such as NMR shielding constants and excitation energies. Then, Moura and co-workers from the Kraka group at Southern Methodist University outline a new protocol called “LMODEAGen” for the determination and analysis of local vibrational modes.<sup>19</sup> This approach avoids chemical intuition in the creation of non-redundant parameter sets and thus provides a unique method to studying larger molecular systems.

Schnack-Petersen and co-workers in the Coriani group at the Technical University of Denmark report a new implementation of the EOM-CC method for resonant inelastic X-ray scattering (RIXS).<sup>20</sup> They find that the second-order approximate CC singles and doubles (CC2) method produces RIXS spectra that are comparable in quality to the more expensive full CC singles and doubles (CCSD) approach. In related work, Konecny et al. working with Ruud and Repisky at the Hylleraas Centre for Quantum Molecular Sciences in Norway have developed a pair of approaches for simulating X-ray absorption spectra (XAS) based on a two-component relativistic framework in the context of TD-DFT.<sup>21</sup> They demonstrate the effectiveness of their

method compared to other approaches using L- and M-edge XAS for transition metal and actinide compounds. In the machine-learning (ML) domain, coupled-cluster-level accuracy from DFT may be possible using well-designed ML models, according to work by Maier, Collins, and Raghavachari at Indiana University.<sup>22</sup> Using an efficient  $\Delta$ -ML model with a systematic molecular fragmentation approach, they report such accuracy for vertical ionization potentials.

## ■ BENCHMARKING STUDIES

The performance of quantum chemical methods must be analyzed systematically in order to judge their reliability and robustness. To that end, Karton at the University of New England in Armidale, Australia, examined the effect of tight  $d$ -type functions in coupled cluster calculations of the atomization energies of a set of 45  $s$ -row species using basis sets of up to sextuple- $\zeta$  quality.<sup>23</sup> He reports that the effects of such functions decline with the overall size of the basis set, but are still significant even at the CCSD(T)/cc-pVQZ level of theory. Opoku, Pawłowski, and Ortiz at Auburn University have benchmarked a set of electron-propagator self-energy approximations using a collection of 55 vertical electron attachment energies of closed-shell anions.<sup>24</sup> They report that new, parameter-free methods provide the basis for a composite procedure that is accurate and provides interpretable results.

Density-functional predictions of electric field gradient tensors have proven to be valuable in the interpretation of solid-state NMR experiments, and Iulucci of Washington and Jefferson College along with Hartman and Beran at the University of California Riverside report their benchmarking study of a dozen beyond-GGA functionals and second-order Møller-Plesset perturbation theory.<sup>25</sup> They find no significant advantages to using double-hybrid functionals or MP2 for the prediction of solid-state NMR chemical shifts vs hybrid functionals.

Quantum computing is also explored in the MQM VSI in work by D’Cunha and Crawford at Virginia Tech and Motta and Rice at IBM Almaden, who examined potential pitfalls of hardware-efficient Ansätze in variational quantum simulations of molecular electronic structure.<sup>26</sup> They report that such methods can yield broken symmetry solutions as well as nondifferentiable potential surfaces, and they offer an analysis that may guide future developments.

## ■ STATE-OF-THE-ART APPLICATIONS OF QUANTUM CHEMISTRY

The ultimate goal of all theoretical and methodological developments in quantum chemistry is to apply the new tools and techniques to important problems in molecular and materials science. North and co-workers in the Wilson group at Michigan State University carried out multireference — complete active space self-consistent field (CASSCF) and MRCI — calculations on lawrencium fluoride and oxide molecules to obtain detailed spectroscopic information for numerous electronic states.<sup>27</sup> In addition, they obtained bond dissociation energies using a range of quantum chemical methods. In work appearing in *J. Phys. Chem. C*, Alessio and co-workers in the Krylov group at the University of Southern California utilized the spin-flip EOM-CC (EOM-SF-CC) method to investigate the magnetic anisotropy of nickelocene in order to benchmark corresponding spin-flip TD-DFT (SF-TD-DFT) calculations.<sup>28</sup> They found good agreement with

experimentally derived values and that the principal contributions to the anisotropy arise from interactions between the triplet ground state and the third singlet state.

Kitzmilller and co-workers in the Schaefer group at the University of Georgia report predictions of the molecular structure and fundamental vibrational frequencies of two formaldehyde analogues based on two elements in the same group as carbon: tin and lead.<sup>29</sup> Using high-level coupled cluster methods combined with focal-point techniques, they provide accurate data intended to guide future experimental detection of these species. In the sole paper of the MQM VSI appearing in section A2, “Aerosols; Environmental and Atmospheric Chemistry; Astrochemistry,” Haney et al. in the Fortenberry group at Ole Miss explore the dependence of the lowest excitation energies of carbonic acid clusters on their dihedral O–C–O–O angles. Their analysis reveals features of potential relevance to the ultimate astrochemical observation of these species.<sup>30</sup> Next, Workman, Firth, and Gichuhi at Tennessee Tech University have simulated the negative-ion photoelectron spectra of three cyano-substituted benzenes.<sup>31</sup> Their results may lead to identification of these species — which are comparable to recently detected cyanonaphthalene and cyanoindene — in the interstellar medium.

Spin–orbit coupling (SOC) in di- and polyradical species can vary considerably with molecular distortions and in the presence of intermolecular interactions. Using restricted active space configuration interaction (RASCI) wave functions, Rodríguez-Jiménez, Carreras, and Casanova at the Donostia International Physics Center in Spain explore the origin of these couplings and introduce a new definition of the SOC constant for molecular aggregates.<sup>32</sup> Next, Villegas-Escobar, Hoobler, Toro-Labbé, and Schaefer at the Pontificia Universidad Católica de Chile and the University of Georgia examined the reactivity of low-valent aluminyl ions toward H<sub>2</sub> through a series of coupled cluster calculations.<sup>33</sup> They found that aluminyl systems with carbon- and nitrogen-based chelating centers would serve well to activate hydrogen without dimerization. Finally, according to a report by Datar, Wright, and Matthews at Southern Methodist University, the presence of electric fields yields shifts in absorption energies and intensities in X-ray Stark spectra that may be attributed to responses in the molecular orbitals, the dipole moment, and the geometry.<sup>34</sup> They also find that both virtual and core orbitals play a role in the observed spectral trends.

The outstanding original articles appearing in this VSI celebrating the 2022 MQM conference are indicative of the breadth and high quality of research ongoing in the field of quantum chemistry. From the development of new methods to their application to chemical grand challenges, molecular electronic structure theory continues to progress as a full partner with experiment in scientific exploration.

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## Notes

Views expressed in this preface are those of the author and not necessarily the views of the ACS.

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