John M. Herbert **April 2025**

Contact

Dept. of Chemistry & Biochemistry
The Ohio State University
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Employment

Professor, The Ohio State University (2014–)

Associate Professor, The Ohio State University (2011–2014)

Assistant Professor, The Ohio State University (2006–2011)

Postdoctoral Fellow, University of California–Berkeley (2004–2006)

- NSF Mathematical Sciences Postdoctoral Fellow
- Advisor: Martin Head-Gordon

Postdoctoral Researcher, The Ohio State University (2003)

- Advisor: Anne McCoy

Education

Ph.D., University of Wisconsin, Madison, WI (1999–2003)

- National Defense Science & Engineering Graduate Fellow
- Advisor: John Harriman
- Thesis: *Reconstructive Approaches to One- and Two-Electron Density Matrix Theory*

B.S., Kansas State University, Manhattan, KS (1994–1999)

- Chemistry and Math double major, including graduate coursework in both
- Graduated *summa cum laude*, with honors (4.0 GPA)
- Thesis: *Ab Initio Vibrational-Rotational Analysis Using Arbitrary-Order Rayleigh-Schrödinger Perturbation Theory in a Computer Algebra Environment*

Awards

- Diversity Enhancement Faculty Award, Ohio State College of Arts & Sciences, 2025
- Charles A. Coulson Lecture, University of Georgia, 2022
- Edward W. Morley Medal, American Chemical Society (Cleveland Section), 2020
- Invited Speaker, 3rd World Laureates Forum (Shanghai, China), 2020
- Alexander von Humboldt Foundation Fellowship, 2016–2017
- ACS *Journal of Physical Chemistry A* Lectureship Award, 2013
- Camille Dreyfus Teacher-Scholar Award, 2011–2016
- ACS Outstanding Junior Faculty Award in Computational Chemistry, 2010
- Alfred P. Sloan Foundation Research Fellowship, 2010–2012.
- Presidential Early Career Award for Scientists and Engineers (PECASE), 2009

- NSF CAREER Award, 2008–2012
- Banned by Gaussian Inc., 2006–present
- NSF Mathematical Sciences Postdoctoral Fellowship, 2004–2006
- IBM/Michael Zerner Award (Sanibel Symposium), 2003
- National Defense Science & Engineering Graduate Fellowship (NDSEG), 1999–2002
- NSF Pre-Doctoral Fellowship, 1999 (declined in favor of NDSEG award)
- Physical Chemistry Graduate Research Award (University of Wisconsin), 2003
- Portz Scholar (National Collegiate Honors Council's Annual Award), 1998
- NSF REU Fellowship (Ohio State University), 1998
- DOE Research Fellowship (Argonne National Laboratory), 1997
- Barry M. Goldwater Scholarship, 1996–1998
- Presidential Scholarship (Kansas State University), 1994–1998

Publications

h-index = 64, total citations = 17,996; 37 papers with $\geq$ 100 citations (source: Google Scholar)

176. M. Gray, A. Mandal, and J. M. Herbert. Revisiting the half-and-half functional. *ChemRxiv* (2025).

175. J. M. Herbert, M. Gray, K.-Y. Liu, and K. Carter-Fenk. Extended symmetry-adapted perturbation theory (XSAPT): A cubic-scaling platform for computing accurate intermolecular interaction energies and *ab initio* energy decomposition analysis. To be published in *Computational Methods for the Analysis of Non-Covalent Interactions*, a volume of *Struct. Bond.* (2025).

174. J. M. Herbert and N. Dickson-Karn. The fallacy of "treating every student the same". *Inside Higher Ed* (March 20, 2025).

173. D. R. Broderick and J. M. Herbert. Untangling sources of error in the density-functional many-body expansion. *J. Phys. Chem. Lett.* **16**, 2793 (2025).

172. A. Mandal and J. M. Herbert. Simplified tuning of long-range corrected time-dependent density functional theory. *J. Phys. Chem. Lett.* **16**, 2672 (2025).

171. P. E. Bowling, M. Gray, S. K. Paul, and J. M. Herbert. Testing a heterogeneous polarizable continuum model against exact Poisson boundary conditions. *J. Chem. Theory Comput.* **21**, 1722 (2025).

170. B. Schramm, M. Gray, and J. M. Herbert. Substituent and heteroatom effects on π–π interactions: Evidence that parallel-displaced π-stacking is not driven by quadrupolar electrostatics. *J. Am. Chem. Soc.* **147**, 3243 (2025).

169. P. E. Bowling, D. R. Broderick, and J. M. Herbert. Quick-and-easy validation of protein–ligand binding models using fragment-based semiempirical quantum chemistry. *J. Chem. Inf. Model.* **65**, 937 (2025).

168. P. E. Bowling, D. R. Broderick, and J. M. Herbert. Convergent protocols for computing protein–ligand interaction energies using fragment-based quantum chemistry. *J. Chem. Theory Comput.* **21**, 951 (2025).

167. D. R. Broderick and J. M. Herbert. Delocalization error poisons the density-functional many-body expansion. *Chem. Sci.* **15**, 19893 (2024).

166. J. M. Herbert and A. Mandal. Importance of orbital invariance in quantifying electron–hole separation and exciton size. *J. Chem. Theory Comput.* **20**, 9446 (2024).

165. J. M. Herbert. Fact-checking the "politicization" of scientific funding. *Chronicle of Higher Education* (October 24, 2024).

164. M. Gray, P. E. Bowling, and J. M. Herbert. Comment on "Benchmarking basis sets for density functional theory thermochemistry calculations: Why unpolarized basis sets and the polarized 6-311G family should be avoided". *J. Phys. Chem. A* **128**, 7739 (2024).

163. M. Gray and J. M. Herbert. Assessing the domain-based local pair natural orbital (DLPNO) approximation for non-covalent interactions in sizable supramolecular complexes. *J. Chem. Phys.* **161**, 054114 (2024).

162. T. Froitzheim, L. Kunze, S. Grimme, J. M. Herbert, and J.-M. Mewes. Benchmarking charge-transfer excited states in TADF emitters: ΔDFT outperforms TD-DFT for emission energies. *J. Phys. Chem. A* **128**, 6324 (2024). (Gustavo Scuseria Festschrift)

161. A. Mandal, E. J. Berquist, and J. M. Herbert. A new parameterization of the DFT/CIS method with applications to core-level spectroscopy. *J. Chem. Phys.* **161**, 044114 (2024).

160. P. E. Bowling, S. Dasgupta, and J. M. Herbert. Eliminating imaginary vibrational frequencies in quantum-chemical cluster models of enzymatic active sites. *J. Chem. Inf. Model.* **64**, 3912 (2024).

159. M. Gray and J. M. Herbert. Density functional theory for van der Waals complexes: Size matters. *Annu. Rep. Comput. Chem.* **20**, 1 (2024).

158. E. Hruska, Q. Zhu, S. Biswas, M. T. Fortunato, D. R. Broderick, C. M. Morales, J. M. Herbert, C. Turro, and L. R. Baker. Water-mediated charge transfer and electron localization in a Co_3Fe_2 cyanide-bridged trigonal bipyramidal complex. *J. Am. Chem. Soc.* **146**, 8031 (2024).

157. J. M. Herbert. Visualizing and characterizing excited states from time-dependent density functional theory. *Phys. Chem. Chem. Phys.* **26**, 3755 (2024).

156. C. J. C. Jordan, M. P. Coons, J. M. Herbert, and J. R. R. Verlet. Spectroscopy and dynamics of the hydrated electron at the water/air interface. *Nat. Commun.* **15**, 182 (2024).

155. A. A. Taka, J. M. Herbert, and L. M. McCaslin. Ground-state orbital analysis predicts S_1 charge transfer in donor–acceptor materials. *J. Phys. Chem. Lett.* **14**, 11063 (2023).

154. D. R. Broderick and J. M. Herbert. Scalable generalized screening for high-order terms in the many-body expansion: Algorithm, open-source implementation, and demonstration. *J. Chem. Phys.* **159**, 174801 (2023). (Special issue: "Modular and Interoperable Software for Chemical Physics".)

153. J. M. Herbert, Y. Zhu, B. Alam, and A. K. Ojha. Time-dependent density functional theory for x-ray absorption spectra: Comparing the real-time approach to linear response. *J. Chem. Theory Comput.* **19**, 6745 (2023).

152. J. M. Herbert. Tackling pedigree bias in faculty hiring. *Inside Higher Ed* (September 27, 2023).

151. V. Gavini, S. Baroni, V. Blum, D. R. Bowler, A. Buccheri, J. R. Chelikowsky, S. Das, W. Dawson, P. Delugas, M. Dogan, C. Draxl, G. Galli. L. Genovese, P. Giannozzi, M. Giantomassi, X. Gonze, M. Govoni, F. Gygi, A. Gulans, J. M. Herbert, S. Kokott, T. K. Kühne, K.-H. Liou, T. Miyazaki, P. Motamarri, A. Nakata, J. E. Pask, C. Plessl, L. E. Ratcliff, R. M. Richard, M. Rossi, R. Schade, M. Scheffler, O. Schütt, P. Suryanarayana, M. Torrent, L. Truflandier, T. L. Windus, Q. Xu, V. W.-Z. Yu, and D. Perez. Roadmap on electronic structure codes in the exascale era. *Model. Simul. Mater. Sci. Eng.* **31**, 063301 (2023).

150. S. Jana and J. M. Herbert. Fractional-electron and transition-potential methods for core-to-valence excitation energies using density functional theory. *J. Chem. Theory Comput.* **19**, 4100 (2023).

149. K. Carter-Fenk and J. M. Herbert. Appraisal of dispersion damping functions for the effective fragment potential method. *Mol. Phys.* **121**, e2055504 (2023). (Peter Gill Festschrift)

148. B. Rana, G. J. O. Beran, and J. M. Herbert. Correcting π-delocalisation errors in conformational energies using density-corrected DFT, with application to crystal polymorphs. *Mol. Phys.* **121**, e2138789 (2023). (Nick Besley Memorial Issue)

147. J. M. Herbert. Density functional theory for electronic excited states. Ch. 3 of *Theoretical and Computational Photochemistry: Fundamentals, Methods, Applications and Synergy with Experimental Approaches*, ed. by C. García-Iriepa and M. Marazzi, pp. 69–118 (Elsevier, 2023).

146. P. E. Bowling, D. R. Broderick, and J. M. Herbert. Fragment-based calculations of enzymatic thermochemistry require dielectric boundary conditions. *J. Phys. Chem. Lett.* **14**, 3826 (2023).

145. J. M. Herbert. Academic free speech or right-wing grievance?. *Digital Discov.* **2**, 260 (2023).

144. S. Jana and J. M. Herbert. Slater transition methods for core-level electron binding energies. *J. Chem. Phys.* **158**, 094111 (2023).

143. M. Gray and J. M. Herbert. Origins of offset-stacking in porous frameworks. *J. Phys. Chem. C* **127**, 2675 (2023).

142. K. Carter-Fenk, B. A. Johnson, J. M. Herbert, G. K. Schenter, and C. J. Mundy. Birth of the hydrated electron via charge-transfer-to-solvent excitation of aqueous iodide. *J. Phys. Chem. Lett.* **14**, 870 (2023).

141. J. M. Herbert and A. Mandal. Spin-flip TDDFT for photochemistry. Ch. 10 of *Time-Dependent Density-Functional Theory: Nonadiabatic Molecular Dynamics*, ed. by C. Zhu pp. 361–404 (Jenny Stanford, 2023).

140. M. Gray, P. E. Bowling, and J. M. Herbert. Systematic evaluation of counterpoise correction in density functional theory. *J. Chem. Theory Comput.* **18**, 67422 (2022).

139. J. M. Herbert, M. Head-Gordon, H. P. Hratchian, T. Head-Gordon, R. E. Amaro, A. Aspuru-Guzik, R. Hoffmann, C. A. Parish, C. M. Payne, and T. Van Voorhis. Words matter: On the debate over free speech, inclusivity, and academic excellence. *J. Phys. Chem. Lett.* **13**, 7100 (2022).

138. B. Rana, M. P. Coons, and J. M. Herbert. Detection and correction of delocalization errors for electron and hole polarons using density-corrected DFT. *J. Phys. Chem. Lett.* **13**, 5275 (2022).

137. Y. Zhu and J. M. Herbert. High harmonic spectra computed using time-dependent Kohn-Sham theory with Gaussian orbitals and a complex absorbing potential. *J. Chem. Phys.* **156**, 204123 (2022).

136. B. Alam, H. Jiang, P. M. Zimmerman, and J. M. Herbert. State-specific solvation for restricted active space spin-flip (RAS-SF) wave functions based on the polarizable continuum formalism. *J. Chem. Phys.* **156**, 194110 (2022).

135. M. Gray and J. M. Herbert. Comprehensive basis-set testing of extended symmetry-adapted perturbation theory and assessment of mixed-basis combinations to reduce cost. *J. Chem. Theory Comput.* **18**, 2308 (2022).

134. A. Ashraf, J. M. Herbert, S. Muhammad, B. A. Farooqi, U. Farooq, M. Salman, and K. Ayub. Theoretical approach to evaluate the gas-sensing performance of graphene nanoribbon/oligothiophene composites. *ACS Omega* **7**, 2260 (2022).

133. J. M. Herbert and S. K. Paul. Interaction energy analysis of monovalent inorganic anions in bulk water versus air/water interface. *Molecules* **26**, 6719 (2021). (Special issue in honor of Frank Weinhold.)

132. K. Carter-Fenk, K. U. Lao, and J. M. Herbert. Predicting and understanding noncovalent interactions using novel forms of symmetry-adapted perturbation theory. *Acc. Chem. Res.* **54**, 3679 (2021).

131. X. Zhang and J. M. Herbert. Nonadiabatic dynamics with spin-flip versus linear-response time-dependent density functional theory: A case study for the protonated Schiff base $C_5H_6NH_2^+$. *J. Chem. Phys.* **155**, 124111 (2021).

130. J. M. Herbert. Neat, simple, and wrong: Debunking electrostatic fallacies regarding noncovalent interactions. *J. Phys. Chem. A* **125**, 7125 (2021).

129. E. Epifanovsky, A. T. B. Gilbert, X. Feng, J. Lee, Y. Mao, N. Mardirossian, P. Pokhilko, A. F. White, M. P. Coons, A. L. Dempwolff, Z. Gan, D. Hait, P. R. Horn, L. D. Jacobson, I. Kaliman, J. Kussmann, A. W. Lange, K. U. Lao, D. S. Levine, J. Liu, S. C. McKenzie, A. F. Morrison, K. D. Nanda, F. Plasser, D. R. Rehn, M. L. Vidal, Z.-Q. You, Y. Zhu, B. Alam, B. J. Albrecht, A. Aldossary, E. Alguire, J. H. Andersen, V. Athavale, D. Barton, K. Begam, A. Behn, N. Bellonzi, Y. A. Bernard, E. J. Berquist, H. G. A. Burton, A. Carreras, K. Carter-Fenk, R. Chakraborty, A. D. Chien, K. D. Closser, V. Cofer-Shabica, S. Dasgupta, M. de Wergifosse, J. Deng, M. Diedenhofen, H. Do, S. Ehlert, P.-T. Fang, S. Fatehi, Q. Feng, T. Friedhoff, J. Gayvert, Q. Ge, G. Gidofalvi, M. Goldey, J. Gomes, C. E. González-Espinoza, S. Gulania, A. O. Gunina, M. W. D. Hanson-Heine, P. H. P. Harbach, A. Hauser, M. F. Herbst, M. Hernández Vera, M. Hodecker, Z. C. Holden, S. Houck, X. Huang, K. Hui, B. C. Huynh, M. Ivanov, Á.Jász, H. Ji, H. Jiang, B. Kaduk, S. Kähler, K. Khistyaev, J. Kim, G. Kis, P. Klunzinger, Z. Koczor-Benda, J. H. Koh, D. Kosenkov, L. Koulias, T. Kowalczyk, C. M. Krauter, K. Kue, A. Kunitsa, T. Kus, I. Ladjánszki, A. Landau, K. V. Lawler, D. Lefrancois, S. Lehtola, R. R. Li, Y.-P. Li, J. Liang, M. Liebenthal, H.-H. Lin, Y.-S. Lin, F. Liu, K.-Y. Liu, M. Loipersberger, A. Luenser, A. Manjanath, P. Manohar, E. Mansoor, S. F. Manzer, S.-P. Mao, A. V. Marenich, T. Markovich, S. Mason, S. A. Maurer, P. F. McLaughlin, M. F. S. J. Menger, J.-M. Mewes, S. A. Mewes, P. Morgante, J. W. Mullinax, K. J. Oosterbaan, G. Paran, A. C. Paul, S. K. Paul, F. Pavošević, Z. Pei, S. Prager, E. I. Proynov, Á. Rák, E. Ramos-Cordoba, B. Rana, A. E. Rask, A. Rettig, R. M. Richard, F. Rob, E. Rossomme, T. Scheele, M. Scheurer, M. Schneider, N. Sergueev, S. M. Sharada, W. Skomorowski, D. W. Small, C. J. Stein, Y.-C. Su, E. J. Sundstrom, Z. Tao, J. Thirman, G. J. Tornai, T. Tsuchimochi, N. M. Tubman, S. P. Veccham, O. Vydrov, J. Wenzel, J. Witte, A. Yamada, K. Yao, S. Yeganeh, S. R. Yost, A. Zech, I. Y. Zhang, X. Zhang, Y. Zhang, D. Zuev, A. Aspuru-Guzik, A. T. Bell, N. A. Besley, K. B. Bravaya, B. R. Brooks, D. Casanova, J.-D. Chai, S. Coriani, C. J. Cramer, G. Cserey, A. E. DePrince III, R. A. DiStasio Jr., A. Dreuw, B. D. Dunietz, T. R. Furlani, W. A. Goddard III, S. Hammes-Schiffer, T. Head-Gordon, W. J. Hehre, C.-P. Hsu, T.-C. Jagau, Y. Jung, A. Klamt, J. Kong, D. S. Lambrecht, W. Liang, N. J. Mayhall, C. W. McCurdy, J. B. Neaton, C. Ochsenfeld, J. A. Parkhill, R. Peverati, V. A. Rassolov, Y. Shao, L. V. Slipchenko, T. Stauch, R. P. Steele, J. E. Subotnik, A. J. W. Thom, A. Tkatchenko, D. G. Truhlar, T. Van Voorhis, T. A. Wesolowski, K. B. Whaley, H. L. Woodcock III, P. M. Zimmerman, S. Faraji, P. M. W. Gill, M. Head-Gordon, J. M. Herbert, and A. I. Krylov. Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *J. Chem. Phys.* **155**, 084801 (2021).

128. B. Rana and J. M. Herbert. Hidden hemibonding in the aqueous hydroxyl radical. *J. Phys. Chem. Lett.* **12**, 8053 (2021).

127. M. Gray and J. M. Herbert. Simplified tuning of long-range corrected density functionals for symmetry-adapted perturbation theory. *J. Chem. Phys.* **155**, 034103 (2021).

126. S. K. Paul and J. M. Herbert. Probing interfacial effects on ionization energies: The surprising banality of anion–water hydrogen bonding at the air/water interface. *J. Am. Chem. Soc.* **143**, 10189 (2021).

125. K. Carter-Fenk, C. J. Mundy, and J. M. Herbert. Natural charge-transfer analysis: Eliminating spurious charge-transfer states in time-dependent density functional theory via diabatization, with application to projection-based embedding. *J. Chem. Theory Comput.* **17**, 4195 (2021).

124. K. A. Carter-Fenk, K. Carter-Fenk, M. A. Fiamingo, H. C. Allen, and J. M. Herbert. Vibrational exciton delocalization precludes the use of infrared intensities as proxies for surfactant accumulation on aqueous surfaces. *Chem. Sci.* **12**, 8320 (2021).

123. J. M. Herbert. Dielectric continuum methods for quantum chemistry. *WIREs Comput. Mol. Sci.* **11**, e1519 (2021).

122. J. M. Herbert and K. Carter-Fenk. Electrostatics, charge transfer, and the nature of the halide–water hydrogen bond. *J. Phys. Chem. A* **125**, 1243 (2021). (Special issue in honor of Dan Neumark.)

121. B. Rana and J. M. Herbert. Role of hemibonding in the structure and ultraviolet spectroscopy of the aqueous hydroxyl radical. *Phys. Chem. Chem. Phys.* **22**, 27829 (2020).

120. B. Alam, A. F. Morrison, and J. M. Herbert. Charge separation and charge transfer in the low-lying excited states of pentacene. *J. Phys. Chem. C* **124**, 24653 (2020).

119. K. Carter-Fenk and J. M. Herbert. Reinterpreting π-stacking. *Phys. Chem. Chem. Phys.* **22**, 24870 (2020).

118. H. Aksu, S. K. Paul, J. M. Herbert, and B. D. Dunietz. How well does a solvated octa-acid capsule shield the embedded chromophore? A computational analysis based on an anisotropic dielectric continuum model. *J. Phys. Chem. B* **124**, 6998 (2020).

117. S. Dasgupta and J. M. Herbert. *Ab initio* approach to femtosecond stimulated Raman spectroscopy: Investigating vibrational modes probed in excited-state relaxation of quaterthiophenes. *J. Phys. Chem. A* **124**, 5356 (2020).

116. K. Carter-Fenk and J. M. Herbert. State-targeted energy projection: A simple and robust approach to relaxation of non-Aufbau self-consistent field solutions. *J. Chem. Theory Comput.* **16**, 5067 (2020).

115. K. Carter-Fenk and J. M. Herbert. Electrostatics does not dictate the slip-stacked arrangement of aromatic π–π interactions. *Chem. Sci.* **11**, 6758 (2020).

114. A. W. Lange, J. M. Herbert, B. J. Albrecht, and Z.-Q. You. Intrinsically smooth discretisation of Connolly's solvent-excluded molecular surface. *Mol. Phys.* **118**, e1644384 (2020).

113. S. Dasgupta and J. M. Herbert. Using atomic confining potentials for geometry optimization and vibrational frequency calculations in quantum-chemical models of enzyme active sites. *J. Phys. Chem. B* **124**, 1137 (2020).

112. T. Jadoon, K. Carter-Fenk, M. B. A. Siddique, J. M. Herbert, R. Hussain, S. Iqbal, J. Iqbal, and K. Ayub. Silver clusters tune up electronic properties of graphene nanoflakes: A comprehensive theoretical study. *J. Mol. Liq.* **297**, 111902 (2020).

111. K.-Y. Liu and J. M. Herbert. Energy-screened many-body expansion: A practical yet accurate fragmentation method for quantum chemistry. *J. Chem. Theory Comput.* **16**, 475 (2020).

110. C. J. Stein, J. M. Herbert, and M. Head-Gordon. The Poisson–Boltzmann model for implicit solvation of electrolyte solutions: Quantum chemical implementation and assessment via Sechenov coefficients. *J. Chem. Phys.* **151**, 224111 (2019).

109. A. Ashraf, K. Carter-Fenk, J. M. Herbert, B. A. Farooqi, U. Farooq, and K. Ayub. Interaction of graphene quantum dots with oligothiophene: A comprehensive theoretical study. *J. Phys. Chem. C* **123**, 29556 (2019).

108. J. M. Herbert. Fantasy versus reality in fragment-based quantum chemistry. *J. Chem. Phys.* **151**, 170901 (2019).

107. S. Dasgupta, B. Rana, and J. M. Herbert. *Ab initio* investigation of the resonance Raman spectrum of the hydrated electron. *J. Phys. Chem. B* **123**, 8074 (2019).

106. J. M. Herbert. Structure of the aqueous electron. *Phys. Chem. Chem. Phys.* **21**, 20538 (2019).

105. K.-Y. Liu, K. Carter-Fenk, and J. M. Herbert. Self-consistent charge embedding at very low cost, with application to symmetry-adapted perturbation theory. *J. Chem. Phys.* **151**, 031102 (2019).

104. J. Liu, B. Rana, K.-Y. Liu, and J. M. Herbert. Variational formulation of the generalized many-body expansion with self-consistent charge embedding: Simple and correct analytic energy gradient for fragment-based *ab initio* molecular dynamics. *J. Phys. Chem. Lett.* **10**, 3877 (2019).

103. K. Carter-Fenk, K. U. Lao, K.-Y. Liu, and J. M. Herbert. Accurate and efficient *ab initio* calculations for supramolecular complexes: Symmetry-adapted perturbation theory with many-body dispersion. *J. Phys. Chem. Lett.* **10**, 2706 (2019).

102. Z. C. Holden, B. Rana, and J. M. Herbert. Analytic gradient for the QM/MM-Ewald method using charges derived from the electrostatic potential: Theory, implementation, and application to *ab initio* molecular dynamics simulation of the aqueous electron. *J. Chem. Phys.* **150**, 144115 (2019).

101. A. F. Morrison, E. Epifanovsky, and J. M. Herbert. Double-buffered, heterogeneous CPU + GPU integral digestion algorithm for single-excitation calculations involving a large number of excited states. *J. Comput. Chem.* **39**, 2173 (2018).

100. K. U. Lao and J. M. Herbert. A simple correction for nonadditive dispersion within extended symmetry-adapted perturbation theory (XSAPT). *J. Chem. Theory Comput.* **14**, 5128 (2018).

99. K. U. Lao and J. M. Herbert. Atomic orbital implementation of extended symmetry-adapted perturbation theory (XSAPT) and benchmark calculations for large supramolecular complexes. *J. Chem. Theory Comput.* **14**, 2955 (2018).

98. M. P. Coons and J. M. Herbert. Quantum chemistry in arbitrary dielectric environments: Theory and implementation of nonequilibrium Poisson boundary conditions and application to compute vertical ionization energies at the air/water interface. *J. Chem. Phys.* **148**, 222834 (2018). (Special issue: "Ions in Water".)

97. Y. Zhu and J. M. Herbert. Self-consistent predictor/corrector algorithms for stable and efficient integration of the time-dependent Kohn-Sham equation. *J. Chem. Phys.* **148**, 044117 (2018).

96. K.-Y. Liu and J. M. Herbert. Understanding the many-body expansion for large systems. III. Critical role of four-body terms, counterpoise corrections, and cutoffs. *J. Chem. Phys.* **147**, 161729 (2017). (Special issue: "From Quantum Mechanics to Force Fields".)

95. S. Bhandari, Z. Zheng, B. Maiti, C.-H. Chuang, M. Porel, Z.-Q. You, V. Ramamurthy, C. Burda, J. M. Herbert, and B. D. Dunietz. What is the optoelectronic effect of the capsule on the guest molecule in aqueous host/guest complexes? A combined computational and spectroscopic perspective. *J. Phys. Chem. C* **121**, 15481 (2017).

94. A. F. Morrison and J. M. Herbert. Analytic derivative couplings and first-principles exciton/phonon coupling constants for an *ab initio* Frenkel-Davydov exciton model: Theory, implementation, and application to compute triplet exciton mobility parameters for crystalline tetracene. *J. Chem. Phys.* **146**, 224110 (2017).

93. K.-Y. Liu, J. Liu, and J. M. Herbert. Accuracy of finite-difference harmonic frequencies in density functional theory. *J. Comput. Chem.* **38**, 1678 (2017).

92. J. M. Herbert and M. P. Coons. The hydrated electron. *Annu. Rev. Phys. Chem.* **68**, 447 (2017).

91. A. F. Morrison and J. M. Herbert. Evidence for singlet fission driven by vibronic coherence in crystalline tetracene. *J. Phys. Chem. Lett.* **8**, 1442 (2017).

90. S. Dasgupta and J. M. Herbert. Standard grids for high-precision integration of modern density functionals: SG-2 and SG-3. *J. Comput. Chem.* **38**, 869 (2017).

89. J.-M. Mewes, J. M. Herbert, and A. Dreuw. On the accuracy of the general, state-specific polarizable-continuum model for the description of correlated ground- and excited states in solution. *Phys. Chem. Chem. Phys.* **19**, 1644 (2017).

88. Z.-Q. You and J. M. Herbert. Reparameterization of an accurate, few-parameter implicit solvation model for quantum chemistry: Composite method for implicit representation of solvent, CMIRS v. 1.1. *J. Chem. Theory Comput.* **12**, 4399 (2016).

87. M. P. Coons, Z.-Q. You, and J. M. Herbert. The hydrated electron at the surface of neat liquid water appears to be indistinguishable from the bulk species. *J. Am. Chem. Soc.* **138**, 10879 (2016).

86. K. U. Lao and J. M. Herbert. Energy decomposition analysis with a stable charge-transfer term for interpreting intermolecular interactions. *J. Chem. Theory Comput.* **12**, 2569 (2016).

85. J. M. Herbert, X. Zhang, A. F. Morrison, and J. Liu. Beyond time-dependent density functional theory using only single excitations: Methods for computational studies of excited states in complex systems. *Acc. Chem. Res.* **49**, 931 (2016).

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Seminars

91. University of Minnesota, Dept. of Chemistry (scheduled for September 2025)
TBA

90. Technical University of Munich (scheduled for June 2025)
TBA

89. Wayne State University, Dept. of Chemistry (scheduled for April 2025)
TBA

88. Wayne State University, Depts. of Chemistry & Biochemistry (scheduled for April 2025)
TBA

87. American Chemical Society, Columbus Section (scheduled for April 2025)
The Way (Chemical) Things Work: A Quantum Chemist's Perspective

86. Rutgers University (Newark), Dept. of Physics (March 2025)
Deconstructing "Meritocracy"

85. Rutgers University (Newark), Dept. of Physics (March 2025)
Fragmentation: A Multiscale Approach to Molecular Electronic Structure

84. Carnegie Mellon University, Dept. of Materials Science & Engineering (October 2024)
Deconstructing Meritocracy: Unpacking Attacks on Diversity, Equity, and Inclusion

83. University of Pittsburgh, Dept. of Chemistry (scheduled for October 2024)
Neat, Simple, and Wrong: "Just-So" Stories About Non-Covalent Interactions

82. University of Richmond, Dept. of Chemistry (January 2024)
Neat, Simple, and Wrong: Just-So Stories Regarding Non-Bonded Interactions

81. Virginia Commonwealth University, Dept. of Chemistry (January 2024)
Neat, Simple, and Wrong: Debunking Non-Covalent Mythology

80. University of Mount Union (Alliance, OH), Dept. of Chemistry (November 2023)
Neat, Simple, and Wrong: Debunking Myths Regarding Non-Bonded Interactions

79. University of Luxembourg, Dept. of Physics & Materials Science (July 2023)
Neat, Simple, and Wrong: Electrostatic Myths Regarding Non-Covalent Interactions

78. University of Pisa, Dept. of Chemistry (July 2023)
Fantasy vs. Reality in Fragment-Based Quantum Chemistry (An Adult Conversation About Fragmentation)

77. The Ohio State University, student chapters of ACS, oSTEM, and FOCUS (April 2023)
Unpacking Attacks on Diversity, Equity, and Inclusivity (DEI) Efforts in Higher Education

76. NOBCChe Collaborative (virtual, January 2023)
Neat, Simple, and Wrong: Electrostatic Fallacies Regarding Non-Covalent Interactions

75. Society of Hispanic Professional Engineers (virtual, September 2022)
Academic Free speech vs. Inclusivity and Diversity (Are They Really in Conflict?)

74. Virginia Tech, Dept. of Chemistry (March 2022)
Neat, Simple, and Wrong: Debunking Electrostatic Myths Regarding Non-Covalent Interactions

73. University of Georgia, Dept. of Chemistry (February 2022)
Neat, Simple, and Wrong: Electrostatic Fallacies Regarding Noncovalent Interactions

72. University of Rostock (Germany), Dept. of Physical & Theoretical Chemistry (virtual, November 2021)
Eliminating Spurious Charge-Transfer States in Condensed-Phase TDDFT

71. Eastern Kentucky University, Dept. of Chemistry & Forensic Science (virtual, September 2021)
Neat, Simple, and Wrong: Debunking Electrostatic Myths Regarding Non-Bonded Interactions

70. Hope College, Dept. of Chemistry (virtual, February 2021)
Neat, Simple, and Wrong: Debunking Some Common Electrostatic Myths Regarding Intermolecular Interactions

69. ACS Cleveland Section (virtual, October 2020)
Extending the Reach of Ab Initio *Quantum Chemistry Via Fragment-Based Approaches*

68. Kent State University (virtual, October 2020)
Neat, Simple, and Wrong: Debunking Electrostatic Myths about Intermolecular Interactions

67. The Ohio State University, Biophysics Program (January 2020)
From Small Things, Big Things Come: Fragment-Based Approaches for Extending the Reach of Quantum Chemistry to Large (Bio)Molecular Systems

66. Academia Sinica (Taipei, Taiwan), Institute for Atomic & Molecular Sciences (December 2019)
Unconventional TD-DFT Methods for Excited States

65. National Chiao Tung University (Hsinchu, Taiwan), Dept. of Chemistry (December 2019)
Fantasy vs. Reality in Fragment-Based Quantum Chemistry

64. NYU Shanghai & East China Normal University (Shanghai, China), Center for Computational Chemistry (December 2019)
Fantasy vs. Reality in Fragment-Based Quantum Chemistry

63. Western Kentucky University, Dept. of Chemistry (May 2019)
From Small Things, Big Things Come: Some Fragment-Based Approaches to Quantum Chemistry

62. ETH Zürich (Switzerland), Dept. of Chemistry & Applied Biosciences (September 2016)
The Hydrated Electron

61. Eötvös Loránd University (Budapest, Hungary), Dept. of Chemistry (September 2016)
The Hydrated Electron

60. University of Bonn (Germany), Mulliken Center for Theoretical Chemistry (June 2016)
Efficient Quantum Chemistry Methods for Non-Covalent Interactions in Many-Body Systems

59. University of Duisburg-Essen (Germany), Dept. of Chemistry (June 2016)
Efficient Quantum Chemistry Methods for Non-Covalent Interactions in Many-Body Systems

58. Max Planck Institute für Kohlenforschung (Mülheim, Germany) (March 2016)
Beyond TDDFT Using Only Single Excitations: Methods for Computational Studies of Excited States in Complex Systems

57. Australian National University (Canberra, Australia), Dept. of Chemistry (April 2015)
Novel Quantum Chemistry Methods for Large Systems: From Non-Covalent Assemblies to Excited-State Energy Transfer

56. University of Sydney (Australia), Dept. of Chemistry (April 2015)
Electronic Structure Theory for Macromolecules & Condensed Phases: DNA, Solvated Electrons, and Beyond

55. University of New South Wales (Sydney, Australia), Dept. of Chemistry (April 2015)
Electronic Structure Theory for Macromolecules & Condensed Phases: DNA, Solvated Electrons, and Beyond

54. National University of Singapore, Dept. of Chemistry (April 2015)
Does the Many-Body Expansion Actually Work?

53. Nanyang Technological University (Singapore), School of Chemistry, Chemical Engineering, & Biotechnology (April 2015)
Electronic Structure in Macromolecules & Condensed Phases: DNA, Solvated Electrons, and Beyond

52. University of Washington, Dept. of Chemistry (February 2015)
Novel Quantum Chemistry Methods for Large Systems: From Non-Covalent Assemblies to Excited-State Energy Transfer

51. University of Wisconsin–Madison, Dept. of Chemistry (February 2015)
Novel Quantum Chemistry Methods for Large Systems: From Non-Covalent Assemblies to Excited-State Energy Transfer

50. University of California–Irvine, Dept. of Chemistry (October 2014)
New Quantum Chemistry Methods for Large(-ish) Systems

49. University of California–Riverside, Dept. of Chemistry (October 2014)
New Quantum Chemistry Methods for Large(-ish) Systems

48. University of California–Merced, Dept. of Chemistry (October 2014)
New Quantum Chemistry Methods for Large(-ish) Systems

47. University of Texas–Austin, Dept. of Chemistry (April 2014)
Fast Electronic Structure Methods for Non-Covalent Interactions

46. University of South Florida, Dept. of Chemistry (February 2014)
The Quantum Chemistry of Intermolecular Interactions: Better, Faster, Cheaper

45. University of Chicago , Dept. of Chemistry (October 2013)
Fast & Accurate Electronic Structure Methods for Intermolecular Interactions

44. Sung Kwun Kwan University (Suwon, South Korea), Dept. of Chemistry (October 2013)
Fast & Accurate Electronic Structure Methods for Intermolecular Interactions

43. Korea Advanced Institute of Science and Technology (Daejeon, South Korea), Dept. of Chemistry (October 2013)
Fast & Accurate Electronic Structure Methods for Intermolecular Interactions

42. Pohang University of Science and Technology (Pohang, South Korea), Dept. of Chemistry (October 2013)
Theoretical Studies of the Hydrated Electron: From Bulk to Clusters

41. Yonsei University (Seoul, South Korea), Dept. of Chemistry (October 2013)
Fast & Accurate Electronic Structure Methods for Intermolecular Interactions

40. Kent State University, Dept. of Chemistry (September 2013)
Fast & Accurate Electronic Structure Methods for Intermolecular Interactions

39. Michigan State University (September 2013)
Fast & Accurate Electronic Structure Methods for Intermolecular Interactions

38. The Ohio State University, Dept. of Chemistry & Biochemistry (August 2013)
Fast & Accurate Electronic Structure Methods for Intermolecular Interactions

37. University of Georgia, Center for Computational Chemistry (March 2013)
Fast & Accurate Electronic Structure Methods for Intermolecular Interactions

36. National Institutes of Health, Laboratory of Computational Biology (March 2013)
Fast & Accurate Electronic Structure Methods for Intermolecular Interactions in Large Systems

35. Washington University (St. Louis), Dept. of Chemistry (October 2012)
Theoretical Studies of the Hydrated Electron: From Bulk to Clusters

34. Academia Sinica (Taipei, Taiwan), Institute for Atomic & Molecular Sciences (September 2012)
Theoretical Studies of the Hydrated Electron: From Bulk to Clusters

33. National Tsing Hua University (Hsinchu, Taiwan), Dept. of Chemistry (September 2012)
Fragmentation Methods for High Accuracy ab Initio *Calculations in Clusters and Large Molecules*

32. Purdue University, Dept. of Chemistry (February 2012)
Electronic Structure in the Condensed Phase: Structure and Spectroscopy of the Hydrated Electron

31. University of Utah, Dept. of Chemistry (February 2012)
Electronic Structure in the Condensed Phase: Structure and Spectroscopy of the Hydrated Electron

30. Auburn University, Dept. of Chemistry (February 2012)
Electronic Structure in Macromolecules & Condensed Phases: DNA, Solvated Electrons, and Beyond

29. Western Kentucky University, Dept. of Chemistry (April 2011)
Electronic Structure in the Condensed Phase: The Important Role of Solvent Polarization

28. University of Louisville, Dept. of Chemistry (April 2011)
Electronic Structure in Macromolecules & Condensed Phases: DNA, Solvated Electrons, and Beyond

27. University of Kansas, Dept. of Chemistry (March 2011)
Electronic Structure in Macromolecules & Condensed Phases: DNA, Solvated Electrons, and Beyond

26. Kansas State University, Dept. of Chemistry (March 2011)
Electronic Structure in Macromolecules & Condensed Phases: DNA, Solvated Electrons, and Beyond

25. Washburn University (Topeka, KS), Dept. of Chemistry (March 2011)
Electronic Structure in Macromolecules & Condensed Phases: DNA, Solvated Electrons, and Beyond

24. Notre Dame University, Dept. of Chemistry (February 2011)
Electronic Structure in Macromolecules & Condensed Phases: DNA, Solvated Electrons, and Beyond

23. Ohio Supercomputer Center, Statewide User Group Meeting (January 2011)
Wave Functions in Water: Toward First-Principles Quantum Mechanics in Liquid Solution

22. The Ohio State University, Dept. of Chemistry (October 2010)
Better, Faster, Cheaper: Bringing Quantum Chemistry to Bear on Macromolecules and Condensed Phases

21. University of Michigan, Dept. of Chemistry (April 2010)
Excited-State Quantum Chemistry for Macromolecules and Condensed Phases: From DNA to Solvated Electrons

20. The Ohio State University, Dept. of Chemistry (March 2010)
Quantum Chemistry for Macromolecules and Condensed Phases

19. Bowling Green State University (Ohio), Dept. of Chemistry (October 2009)
Excited-State Quantum Chemistry for Macromolecules and Condensed Phases

18. Wright State University (Dayton, Ohio), Dept. of Chemistry (September 2009)
Excited-State Quantum Chemistry for Macromolecules and Condensed Phases

17. University of Wisconsin–Madison, Theoretical Chemistry Institute (April 2008)
Trouble with TDDFT: A Public Service Announcement about Large-Scale Excited-State Calculations (Including DNA)

16. University of Cincinnati, Dept. of Chemistry (March 2008)
Trouble with TDDFT: A Public Service Announcement about Large-Scale Excited-State Calculations

15. Cleveland State University, Dept. of Chemistry (March 2008)
Trouble with TDDFT: A Public Service Announcement about Large-Scale Excited-State Calculations

14. University of Southern California, Dept. of Chemistry (December 2007)
Electron Correction Effects in $(H_2O)_n^-$ and Implications for Modeling of Solvated Electrons

13. Arizona State University, Dept. of Chemistry & Biochemistry (February 2006)
Structure, Electron Correlation, and Excess-Electron Dynamics in Solvated-Electron Clusters, $(H_2O)_n^-$

12. University of Pennsylvania, Dept. of Chemistry (January 2006)
Structure, Electron Correlation, and Excess-Electron Dynamics in Solvated-Electron Clusters, $(H_2O)_n^-$

11. Penn State, Dept. of Chemistry (January 2006)
Structure, Electron Correlation, and Excess-Electron Dynamics in Solvated-Electron Clusters, $(H_2O)_n^-$

10. University of Delaware, Dept. of Chemistry (January 2006)
Structure, Electron Correlation, and Excess-Electron Dynamics in Solvated-Electron Clusters, $(H_2O)_n^-$

9. University of Utah, Dept. of Chemistry (January 2006)
Structure, Electron Correlation, and Excess-Electron Dynamics in Solvated-Electron Clusters, $(H_2O)_n^-$

8. Harvard University, Dept. of Chemistry (December 2005)
Structure, Electron Correlation, and Excess-Electron Dynamics in Solvated-Electron Clusters, $(H_2O)_n^-$

7. University of California–Riverside, Dept. of Chemistry (December 2005)
Structure, Electron Correlation, and Excess-Electron Dynamics in Solvated-Electron Clusters, $(H_2O)_n^-$

6. Syracuse University, Dept. of Chemistry (December 2005)
   Structure, Electron Correlation, and Excess-Electron Dynamics in Solvated-Electron Clusters, $(H_2O)_n^-$

5. The Ohio State University, Dept. of Chemistry (November 2005)
   Structure, Electron Correlation, and Excess-Electron Dynamics in Solvated-Electron Clusters, $(H_2O)_n^-$

4. University of Pittsburgh, Dept. of Chemistry (November 2005)
   Structure, Electron Correlation, and Excess-Electron Dynamics in Solvated-Electron Clusters, $(H_2O)_n^-$

3. University of California–Los Angeles, Dept. of Chemistry (November 2004)
   Efficient, Linear-Scaling Electronic Structure Theory and Its Extension to ab Initio *Molecular Dynamics*

2. University of California–Berkeley, Lester research group (November 2004)
   Density Matrix Methods for Linear-Scaling Self-Consistent Field Theory and ab Initio *Molecular Dynamics*

1. The Ohio State University, Dept. of Chemistry (November 2003)
   Density Matrix *Functional Theory and Long-Range Electron Correlation*

Conference Presentations (Invited)

128. International Chemical Congress of Pacific Basin Societies ("Pacifichem"), Symposium on "Computational Quantum Chemistry: Synergy Between Theory and Experiment" in Honor of Peter Gill
   ◦ Honolulu, HI (scheduled for December 2025)
   ◦ *Importance of Orbital Invariance in Measuring Electron–Hole Separation and Exciton Size*

127. ACS National Meeting, PHYS Division Symposium on "Embedding Methods for Ground and Excited States"
   ◦ Washington, DC (scheduled for August 2025)
   ◦ *Open-Source Framework for Fragment-Based Quantum Chemistry*

126. Talking Politics Special Roundtable: Examining (Anti-)Wokeism Beyond Borders
   ◦ virtual (February 2025)
   ◦ *Standing Up for DEI*

125. 11th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP), Symposium on "Low-Order Scaling Methods for Electronic Structure"
   ◦ Qingdao, China (October 2024)
   ◦ *An Open-Source Framework for Fragment-Based Quantum Chemistry*

124. Q-Chem User Workshop
   ◦ Qingdao, China (October 2024)
   ◦ *Upcoming Q-Chem Features*

123. Q-Chem User Workshop
   ◦ Qingdao, China (October 2024)
   ◦ *Introduction to Q-Chem*

122. 30th Canadian Symposium on Theoretical and Computational Chemistry
   ◦ Halifax, Nova Scotia (July 2024)
   ◦ *How Accurate is DFT for Nanoscale van der Waals Complexes, and What Are the Alternatives?*

121. TSRC Workshop, "Many-Body Interactions: From Quantum Mechanics to Force Fields"
    - Telluride, CO (June 2024)
    - *High-Order Many-Body Expansions via Energy-Based Screening*

120. TSRC Workshop, "Spatio-Temporal Dynamics of Excitons: Bridging the Gap Between Quantum Mechanics and Applications"
    - Telluride, CO (June 2024)
    - *The Importance of Orbital Invariance in Measuring Electron–Hole Separation*

119. 35th International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences (Math/Comp/Chem)
    - Dubrovnik, Croatia (June 2024)
    - *High-Fidelity Fragmentation Methods in Quantum Chemistry*

118. Midwest Theoretical Chemistry Conference
    - Madison, WI (May 2024)
    - *High-Fidelity Fragmentation Methods in Quantum Chemistry*

117. ACS National Meeting, COMP Division, Computers in Chemical & Pharmaceutical Research Award Symposium
    - New Orleans, LA (March 2024)
    - *Accurate QM for Large Supramolecular Complexes: How Good Is DFT and What Are the Other Options?*

116. Institute for Computational Molecular Science, Summer School on DFT
    - Boise State University (June 2023)
    - *Molecular DFT and TD-DFT* (6 lectures)

115. TSRC Workshop, "Intermolecular Interactions: New Challenges for *ab Initio* Theory"
    - Telluride, CO (March 2023)
    - *Investigation of π-Stacking Interactions with XSAPT+MBD*

114. ACS National Meeting, COMP Division Symposium on "QM/QM and Embedding Models"
    - Indianapolis, IN (March 2023)
    - *Simple, Accurate, and Robust Fragmentation Approaches for Quantum Chemistry*

113. CECAM Winter School on Computational Chemistry
    - virtual (February 2023)
    - *Solvation Models in Q-Chem (for Ground and Excited States)*

112. New Horizons in Scientific Software (NHISS-2022)
    - Jeju Island, South Korea (December 2022)
    - *High-Fidelity Fragmentation Approximations for Quantum Chemistry*

111. TSRC Workshop, "Spatio-Temporal Dynamics of Excitons: Bridging the Gap Between Quantum Mechanics and Applications"
    - Telluride, CO (September 2022)
    - *Diagnosing Delocalization Error Using Density-Corrected DFT*

110. ACS National Meeting, PHYS Division Symposium on "Quantum Chemistry: Current and Future Frontiers"
    - Chicago, IL (August 2022)
    - *Predicting and Understanding Noncovalent Interactions Using Novel Forms of Symmetry-Adapted Perturbation Theory*

109. Gordon Research Conference on Molecular and Ionic Clusters
    - Lucca, Italy (August 2022)
    - *Anions at the Air/Water Interface*

108. 12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC)
    - Vancouver, Canada (July 2022)
    - *Reinterpreting π-Stacking*

107. 10th Triennal Conference on Molecular Quantum Mechanics (MQM)
    - Blacksburg, VA (June 2022)
    - *XSAPT (Extended Symmetry-Adapted Perturbation Theory)*

106. Theory and Simulation of Electronic and Optical Processes in Molecules and Materials
    - virtual (February 2022)
    - *Unpaired Spins in Condensed-Phase DFT*

105. CECAM Workshop, "Advances in Electrostatic Calculations: The Road Towards the Exascale"
    - virtual (September 2021)
    - *Poisson Equation Boundary Conditions for Quantum Chemistry*

104. 17th International Conference on Computational Methods in Sciences and Engineering, Symposium on "Quantum Science"
    - virtual (September 2021)
    - *Debunking Electrostatic Myths Concerning Noncovalent Interactions: Qualitative Insight from Quantitative Calculations*

103. CECAM Workshop, "Non-Covalent Interactions in Large Molecules and Extended Materials"
    - virtual (August 2021)
    - *Quantitative Calculations and Qualitative Insight from Cubic-Scaling Variants of Symmetry-Adapted Perturbation Theory*

102. Dept. of Energy, Computational and Theoretical Chemistry Program Meeting
    - virtual (August 2021)
    - *Accurate Energy Decomposition for Noncovalent Interactions: Qualitative Insight from Quantitative Calculations*

101. TSRC Workshop, "Spatio-Temporal Dynamics of Excitons: Bridging the Gap Between Quantum Mechanics and Applications"
    - virtual (June 2021)
    - *Charge Separation in the Low-Lying Excited States of Pentacene*

100. ACS National Meeting, PHYS Division Symposium on "Dynamics of Chemical Reactions from Gas Phase to Interfaces, A Symposium in Honor of Professor William L. Hase"
    - virtual (April 2021)
    - *Interfacial Effects on Ionization Energies and the Surprising Banality of Anion–Water Hydrogen Bonding at the Air/Water Interface*

99. CUNY Graduate Center Initiative on Theoretical Sciences, Symposium on "Spatio-Temporal Dynamics of Excitons: Bridging the Gap Between Quantum Mechanics and Applications"
    - virtual (November 2020)
    - *Charge-Transfer States in Pentacene, from Dimer to Crystal*

98. World Laureates Association, Young Scientists' Forum
    - virtual (October 2020)
    - *Extending the Reach of* Ab Initio *Quantum Chemistry to Macromolecules*

97. 11th Xiamen Workshop on Surface Chemistry, Symposium on "Excited-State Electronic Structure and Dynamics Theories of Complex Systems"
    - Xiamen, China (December 2019)
    - *Spin-Flip TDDFT for Photochemistry*

96. Utah Workshop on Quantum Methods in Molecular and Solid-State Theory
    - Park City, UT (September 2019)
    - *XSAPT: Symmetry-Adapted Perturbation Theory for Many-Body Systems*

95. Workshop on "TDDFT—Excited States and Dynamics"
    - Rutgers University (August 2019)
    - *Hydrated Electron at the Air/Water Interface*

94. Midwest Undergraduate Computational Chemistry Conference (MU3C)
    - The Ohio State University (July 2019)
    - *Quantum Chemistry of Noncovalent Interactions*

93. TSRC Workshop, "Quantum Dynamics and Spectroscopy in Condensed-Phase Materials and Bio-Systems"
    - Telluride, CO (June 2019)
    - *Vibronic Coherence in Singlet Fission: Results from an ab Initio Exciton Model*

92. Mathematics of Finite Elements and Applications (MAFELAP), Symposium on "Numerical Methods for Continuum Solvation"
    - Brunel University, London, UK (June 2019)
    - *Dielectric Continuum Solvation in Quantum Chemistry*

91. Dept. of Energy, Computational and Theoretical Chemistry Program Meeting
    - Gaithersburg, MD (May 2019)
    - *Recent Developments in Fragment-Based Quantum Chemistry*

90. ACS National Meeting, PHYS Division Symposium on "Quantum Embedding Electronic Structure Methods"
    - Orlando, FL (April 2019)
    - *Electrostatically-Embedded Fragment Method with Simple (and Correct!) Analytic Gradients*

89. Workshop on "Emerging Tools for Designing Practical Next Generation Catalysts"
    - Texas A&M University-Qatar, Doha, Qatar (March 2019)
    - *Mechanistic Aspects of Singlet Fission Studied with a First-Principles Exciton Model*

88. Mini-Symposium on Electronic Structure Theory
    - University of California, Berkeley, CA (December 2018)
    - *Hydrated Electron at the Air/Water Interface*

87. ACS National Meeting, PHYS Division Symposium on "Characterization, Detection, and Application of Excitons in Chemistry"
    - Boston, MA (August 2018)
    - *Vibronic Coherence in Singlet Fission: Results for Crystalline Tetracene from an ab Initio Exciton Model*

86. ACS National Meeting, PHYS Division Symposium on "Recent Advances in DFT & TDDFT: Theory and Simulations"
    - Boston, MA (August 2018)
    - *Self-Consistent Predictor/Corrector Algorithms for Provably Stable Propagation of the Time-Dependent Kohn-Sham Orbitals*

85. TSRC Workshop, "Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems: Methods and Applications"
    - Telluride, CO (July 2018)
    - *Quantum Chemistry in Arbitrary Dielectric Environments*

84. TSRC Workshop, "Developments in QM/MM and Embedding Models for Photochemical and Electron Transfer Processes"
    - Telluride, CO (July 2018)
    - *Quantum Chemistry in Arbitrary Dielectric Environments*

83. Dept. of Energy, Computational and Theoretical Chemistry Program Meeting
    - Gaithersburg, MD (May 2018)
    - Ab Initio *Exciton Models*

82. 11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC)
    - Munich, Germany (August 2017)
    - *First-Principles Exciton Models, with Application to Singlet Fission*

81. Q-Chem User Workshop
    - Munich, Germany (August 2017)
    - *Advanced Q-Chem Features*

80. ACS National Meeting, PHYS Division Symposium on "Electronic Structure of Complex Chemical Systems"
    - Washington, DC (August 2017)
    - *First-Principles Exciton Models, with Application to Singlet Fission*

79. Workshop on "Intermolecular Interactions: New Challenges for *ab Initio* Theory"
    - Arenas de Cabrales, Spain (July 2017)
    - *Energy Decomposition Analysis Using Kohn-Sham-based SAPT and Constrained DFT*

78. Q-Chem User Workshop
    - RIKEN Research Institute, Tokyo, Japan (June 2017)
    - *A Preview of Q-Chem v. 5*

77. Q-Chem User Workshop
    - Dalian, China (June 2017)
    - *A Preview of Q-Chem v. 5*

76. 57th Sanibel Symposium
    - St. Simons Island, GA (February 2017)
    - *First-Principles Exciton Models*

75. Energy, Materials, Nanotechnology (EMN) Conference, Symposium on "Novel Electron Correlation Methods for Complex Systems"
    - Las Vegas, NV (October 2016)
    - Ab Initio *Exciton Models*

74. Energy, Materials, Nanotechnology (EMN) Conference, Symposium on "Density Functional Theory and Its Applications"
    - Las Vegas, NV (October 2016)
    - *TDDFT for Photochemistry*

73. ACS National Meeting, PHYS Division Symposium on "Advanced Potential Energy Surfaces"
    - Philadelphia, PA (August 2016)
    - *Spin-Flip Time-Dependent Density Functional Theory for Exploring Excited-State Potential Energy Surfaces*

72. Penn Conference on Theoretical Chemistry
    - University of Pennsylvania (August 2016)
    - *Conical Intersections and Spin-Flip TDDFT*

71. 9th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP), Symposium on "Complex Systems"
    - Grand Forks, ND (July 2016)
    - *Symmetry-Adapted Perturbation Theory for Many-Body Systems*

70. TSRC Workshop, "Ions in Solution: Biology, Energy, and Environment"
    - Telluride, CO (July 2016)
    - *The Solvated Electron*

69. Workshop on "On-the-Fly *ab Initio* Dynamics"
    - City University of New York (May 2016)
    - *Density Functional Theory for Excited-State Potential Energy Surfaces*

68. Dept. of Energy, Computational and Theoretical Chemistry Program Meeting
    - Annapolis, MD (May 2016)
    - *Fragment-Based Quantum Chemistry for Non-Covalent Interactions and Excitation Energy Transfer*

67. 12th International Conference on Computational Methods in Sciences and Engineering (ICCMSE), Symposium on "Computational Chemistry"
    - Athens, Greece (March 2016)
    - *Beyond TDDFT Using Only Single Excitations: Methods for Computational Studies of Excited States in Complex Systems*

66. ACS National Meeting, PHYS Division Symposium on "Time-Dependent Dynamics and Electronic Excited States"
    - San Diego, CA (March 2016)
    - *New Computational Tools for Photochemistry, Solvatochromatic Shifts, and Excitation Energy Transfer*

65. 3rd Annual DOE/NSF Materials Genome Initiative Principal Investigators' Meeting
    - Bethesda, MD (January 2016)
    - *Fragment-Based Quantum Chemistry for Non-Covalent Interactions and Excitation Energy Transfer*

64. International Chemical Congress of Pacific Basin Societies ("Pacifichem"), Symposium on "Practical Strategies for Modeling Non-Covalent Interactions"
    - Honolulu, HI (December 2015)
    - *Recent Developments in the XSAPT Methodology*

63. Workshop on "Multiple Faces of Biomolecular Electrostatics"
    - Mathematical Biosciences Institute, The Ohio State University (October 2015)
    - *What Can Quantum-Inspired Electrostatics Methods Contribute to Biomolecular Applications?*

62. Quantum Systems in Chemistry and Physics (QSCP XX)
    - Varna, Bulgaria (September 2015)
    - *New SCF-Based Methods for Excited States: Conical Intersections and Excitation Energy Transfer*

61. ACS National Meeting, PHYS Division Symposium for Undergraduates
    - Boston, MA (August 2015)
    - *Electronic Structure Theory for Large Systems*

60. TSRC Workshop, "Nonequilibrium Phenomena, Nonadiabatic Dynamics, and Spectroscopy"
    - Telluride, CO (July 2015)
    - *Analytic Derivative Couplings for Time-Dependent DFT*

59. TSRC Workshop, "Excited States: Electronic Structure and Dynamics"
    - Telluride, CO (July 2015)
    - *New Methods Based on Time-Dependent DFT: Conical Intersections and Excitation Energy Transfer*

58. TSRC Workshop, "Intermolecular Interactions: New Challenges for *ab Initio* Theory"
    - Telluride, CO (July 2015)
    - *Recent Developments in the XSAPT Methodology*

57. Dept. of Energy, Computational and Theoretical Chemistry Program Meeting
    - Annapolis, MD (April 2015)
    - *Accurate and Efficient Quantum Chemistry Methods for Non-Covalent Interactions*

56. ACS National Meeting, PHYS Division Symposium on "Modeling Excited States of Complex Systems"
    - Denver, CO (March 2015)
    - *New Electronic Structure Methods for Describing Excited States in Multi-Chromophore and Other Large Systems*

55. ACS National Meeting, PHYS Division Symposium on "Electronic Structure Methods for Highly Polarizable Systems"
    - Denver, CO (March 2015)
    - *An ab Initio Implementation of the Frenkel-Davydov Exciton Model*

54. 2nd Annual DOE/NSF Materials Genome Initiative Principal Investigators' Meeting
    - Bethesda, MD (January 2015)
    - *Efficient Methods for Computing High-Accuracy Non-Covalent Interaction Energies in Clusters, Liquids, and Molecular Crystals*

53. Quantum Systems in Chemistry and Physics (QSCP XIX)
    - Tapei, Taiwan (November 2014)
    - *New DFT-Based Methods for Excited States*

52. International Conference on Chemical Bonding
    - Kauai, HI (July 2014)
    - *Theoretical Studies of the Hydrated Electron in Clusters, Bulk Water, and the Air/Water Interface*

51. Gordon Research Conference on Atomic and Molecular Interactions
    - Easton, MA (July 2014)
    - *Does the Many-Body Expansion Actually Work?*

50. TSRC Workshop, "Ions in Solution and Molecular Biology: Theory, Modeling, and Experiment"
    - Telluride, CO (July 2014)
    - *Structure and Spectroscopy of the Bulk and Interfacial Hydrated Electron*

49. TSRC Workshop, "Spectroscopy and Dynamics on Multiple Potential Surfaces
    - Telluride, CO (July 2014)
    - *Low-Cost DFT-Based Methods for Locating and Describing Conical Intersections*

48. Conference on Excited State Processes
    - Santa Fe, NM (June 2014)
    - *Electronic Structure Methods for Excited States of Molecular Aggregates and Assemblies of Chromophores*

47. Gordon Research Conference on Molecular and Ionic Clusters
    - Lucca, Italy (April 2014)
    - *New Theoretical Methods for Computing Interactions in Large Ionic Molecular Clusters*

46. Southeastern ACS Regional Meeting (SERMACS), Symposium on "Electronic Structure in Complex Environments"
    - Atlanta, GA (November 2013)
    - *XSAPT: A Fast and Accurate Method for Incorporating Explicit Solvent Molecules*

45. Korean Chemical Society National Meeting
    - Changwon, Korea (October 2013)
    - *Fragment and Monomer-Based Methods for Large Scale (and Accurate!) Quantum Chemistry*

44. Mini-Symposium on Electronic Structure Theory
    - University of California, Berkeley, CA (October 2013)
    - *Efficient Monomer-Based Electronic Structure Methods for Intermolecular Interactions*

43. ACS National Meeting, PHYS Division Awards Symposium
    - Indianapolis, IN (September 2013)
    - *Fast & Accurate Electronic Structure Methods for Intermolecular Interactions in Large Systems*

42. ACS National Meeting, PHYS Division Symposium on "Theory and Experiment on Water and Hydration"
    - Indianapolis, IN (September 2013)
    - *Theoretical Studies of the Hydrated Electron*

41. Dept. of Energy, Predictive Theory and Modeling for the Materials Genome Initiative
    - Bethesda, MD (July 2013)
    - *Fast and Accurate ab Initio Methods for Intermolecular Interactions*

40. TSRC Workshop, "Intermolecular Interactions: New Challenges for *ab Initio* Theory"
    - Telluride, CO (July 2013)
    - *Efficient Monomer-Based Methods for Computing Intermolecular Interactions in Many-Body Systems*

39. Midwest Theoretical Chemistry Conference
    - Urbana-Champaign, IL (May 2013)
    - *Accurate Quantum Chemistry for Non-Covalent Interactions in Large Systems*

38. Workshop on "Charge Transfer on the Nanoscale"
    - Brookhaven National Lab (May 2013)
    - *Theoretical Studies of the Structure and Spectroscopy of the Hydrated Electron*

37. Gordon Research Conference on Molecular Energy Transfer
    - Ventura, CA (January 2013)
    - *Fragmentation Methods for High Accuracy ab Initio Calculations in Large Molecular and Ionic Clusters*

36. DOE Nanoporous Materials Genome Center Kick-Off Meeting
    - Minneapolis, MN (November 2012)
    - *Development of Accurate & Affordable Electronic Structure Methods for the Condensed Phase*

35. Dreyfus Foundation Symposium on "Research Frontiers in the Chemical Sciences"
    - New York, NY (October 2012)
    - *Fragmentation Methods for High Accuracy ab Initio Calculations in Clusters and Large Molecules*

34. 1st International Conference on Material Chemistry: Theoretical, Computational, and Experimental Perspectives
    - Taipei, Taiwan (September 2012)
    - *Fragmentation Methods for High Accuracy ab Initio Calculations in Clusters and Large Molecules*

33. ACS National Meeting, PHYS Division Symposium on "Photochemistry in Biology"
    - Philadelphia, PA (August 2012)
    - *TD-DFT Studies of Excited States of DNA Model Systems*

32. ACS National Meeting, PHYS Division Symposium on "Electron and Energy Transfer Phenomena: At the Intersection of Electronic Structure Theory and Chemical Dynamics"
    - Philadelphia, PA (August 2012)
    - *Nailing Down the Energetics of the Aqueous Electron*

31. ACS National Meeting, PHYS Division Symposium on "Bridging the Gap Between *Ab Initio* and Classical Simulations"
    - Philadelphia, PA (August 2012)
    - *Some Bridges between Classical and Quantum Chemical Simulation*

30. Q-Chem User Workshop
    - Philadelphia, PA (August 2012)
    - *Polarizable Continuum Models in Q-Chem*

29. TSRC Workshop, "Ions in Aqueous Solutions and Molecular Biology: Theory, Simulation, and Modeling"
    - Telluride, CO (July 2012)
    - *Structure, Energetics, and Spectroscopy of $e^-(aq)$: The Important Role of Solvent Polarization*

28. TSRC Workshop, "Interfacial Molecular and Electronic Structure and Dynamics"
    - Telluride, CO (July 2012)
    - *Structure and Energetics of $e^-(aq)$ and $(H_2O)_n^-$ According to a Polarizable One-Electron Model*

27. Astrobiology Science Conference, Symposium on "The Role of UV Radiation in Prebiotic Chemistry"
    - Atlanta, GA (April 2012)
    - *Nailing Down the Energetics of the Aqueous Electron*

26. 7th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP)
    - Tokyo, Japan (September 2011)
    - *Structure and Spectroscopy of the Hydrated Electron: Polarizable QM/MM Results*

25. ACS National Meeting, PHYS Division Symposium on "Reduced Density Matrices in Quantum Chemistry"
    - Denver, CO (August 2011)
    - *First-Principles, Fragment-Based Self-Consistent Field Method with a Perturbative Treatment of Intermolecular Interactions: "XPol + SAPT"*

24. ACS National Meeting, PHYS Division Symposium for Undergraduates
    - Denver, CO (August 2011)
    - *Excited-State Dynamics: Theory and Experiment*

23. ACS Central Regional Meeting, Symposium on "The New Frontier of Combined Quantum Mechanical Molecular Mechanical Methods: Theory and Applications in Chemistry and Biology"
    - Indianapolis, IN (June 2011)
    - *Structure, Dynamics, and Spectroscopy of the Hydrated Electron: The Role of Solvent Polarization*

22. ACS National Meeting, PHYS Division Symposium on "Fragment and Local Orbital Methods in Electronic Structure Theory"
    - Anaheim, CA (March 2011)
    - *First-Principles, Fragment-Based Self-Consistent Field Method with a Perturbative Treatment of Intermolecular Interactions: "XPol + SAPT"*

21. Q-Chem Developers' Meeting
    - Anaheim, CA (March 2011)
    - *New Developments in "Polarizable Continuum" Implicit Solvent Models for QM, MM, and QM/MM Applications*

20. Molecular and Ionic Clusters Conference
    - Niigata, Japan (September 2010)
    - *Structure and Spectroscopy of the Hydrated Electron: The Importance of Self-Consistent Polarization*

19. ACS National Meeting, PHYS Division Symposium on "Electrons in Biomolecules"
    - Boston, MA (August 2010)
    - *The Role of Solvent Polarization in the Spectroscopy of $e^-(aq)$*

18. Gordon Research Conference on Atomic and Molecular Interactions
    - Colby-Sawyer College, NH (July 2010)
    - *Photoelectron & Photoionization Dynamics*

17. TSRC Workshop, "Spectroscopy and Dynamics on Multiple Potential Surfaces"
    - Telluride, CO (July 2010)
    - *The Role of Solvent Polarization in the Spectroscopy of $e^-(aq)$*

16. 16th German-American Frontiers of Science Symposium
    - Potsdam, Germany (June 2010)
    - *Quantum Chemistry for Macromolecules and Condensed Phases: From Solvated Electrons to DNA*

15. 6th Triennal Conference on Molecular Quantum Mechanics (MQM)
    - Berkeley, CA (May 2010)
    - *The Role of Self-Consistent Polarization in QM/MM Calculations: The Hydrated Electron as a Test Case*

14. ACS National Meeting, PHYS Division Symposium on "Dynamics in Clusters and Floppy Systems: Theory and Experiment"
    - San Francisco, CA (March 2010)
    - *Structure & Spectroscopy of the Hydrated Electron: Results from a New One-Electron Model, with Self-Consistent Polarization*

13. Gordon Research Conference on Electronic Spectroscopy and Dynamics
    - Colby College, ME (July 2009)
    - *Excited-State Quantum Chemistry for Macromolecules and Condensed Phases*

12. Q-Chem User Workshop
    - Pittsburgh Supercomputer Center (March 2009)
    - *Calculation and Characterization of Excited States Using TD-DFT*

11. Workshop on "Chemical Dynamics: Challenges and Approaches"
    - Institute for Mathematics and Its Applications, University of Minnesota (January 2009)
    - *A Polarizable, Fourier-Grid QM/MM Model for $(H_2O)_N^-$*

10. ACS National Meeting, PHYS Division Symposium on "Spectroscopic Probes of Chemical Dynamics in Gaseous and Condensed Phases"
    - Philadelphia, PA (August 2008)
    - *Using Theory to Make a Direct Connection between Interaction Potentials and Spectroscopy*

9. 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP), Symposium in honor of Ernest Davidson
    - Vancouver, Canada (July 2008)
    - *Unraveling the Excited States of DNA Multimers Using Long-Range-Corrected TD-DFT*

8. CCP6 Workshop on "Potential Energy Surfaces in Many Dimensions"
   - University of Aberdeen, Scotland (July 2008)
   - *The Role of the* Neutral *Water Potential in Determining the Properties of Anionic Water Clusters,* $(H_2O)_n^-$

7. TSRC Workshop, "Spectroscopy and Dynamics on Multiple Potential Surfaces"
   - Telluride, CO (July 2008)
   - *Unravelling the Excited States of DNA Multimers Using Time-Dependent DFT*

6. ACS National Meeting, PHYS Division Symposium on "Electronic Structure and Reaction Dynamics of Open-Shell Species: Theory and Experiment"
   - New Orleans, LA (April 2008)
   - *Adjusting the Knobs on the Hydrated-Electron Pseudopotential*

5. 48th Sanibel Symposium
   - St. Simons Island, GA (February 2008)
   - *Ab Initio and not-so-ab-Initio Approaches to Simulation of the Hydrated Electron*

4. ACS National Meeting, PHYS Division Symposium on "Hydration: From Clusters to Aqueous Solution"
   - Boston, MA (August 2007)
   - *Ab Initio Calculations of Hydrated Electron Clusters,* $(H_2O)_n^-$*: Electron Correlation, Electron Penetration, and Vibrational Spectroscopy*

3. ACS National Meeting, PHYS Division Symposium on "Frontiers in Molecular Dynamics: Experiment and Theory"
   - San Francisco, CA (September 2006)
   - *Is the Carr-Parrinello trick necessary in Gaussian basis sets?*

2. TSRC Workshop, "Spectroscopy and Dynamics on Multiple Potential Surfaces"
   - Telluride, CO (July 2006)
   - *Spectroscopy of Small Water Cluster Anions,* $(H_2O)_n^-$

1. National Collegiate Honors Conference
   - Chicago, IL (November 1998)
   - *Cooperation and Conflict with Imperfect Communication: Prisoner's Dilemma with Noise*

Conference Presentations (Contributed)

51. Penn Conference on Theoretical Chemistry
    - Philadelphia, PA (scheduled for May 2025)
    - *Self-Interaction Error and the DFT-Based Many-Body Expansion*

50. ACS National Meeting, COMP Division Symposium on "Quantum Mechanics"
    - San Diego, CA (March 2025)
    - *Critical Evaluation of Charge-Transfer Diagnostics for TD-DFT Calculations*

49. ACS National Meeting, PHYS Division Symposium on "Open-Source Software in Physical Chemistry"
    - Denver, CO (August 2024)
    - *Open-Source Framework for Community Validation of Fragment-Based Quantum Chemistry*

48. ACS National Meeting, PHYS Division Symposium on "Addressing the Complexity of Correlated Quantum Many-Body Problems by Embedding and Downfolding"
    - Denver, CO (August 2024)
    - *Automated Determination of Active Molecular Orbitals for Solution-Phase Embedding Calculations*

47. ACS National Meeting, COMP Division Symposium on "Quantum Mechanics"
    - San Francisco, CA (August 2023)
    - *High-Order Many-Body Expansions via a Bottom-Up Algorithm*

46. ACS National Meeting, COMP Division Symposium on "Free and Open Source Software: Harnessing the Power of Data"
    - San Francisco, CA (August 2023)
    - *An Open-Source Framework for Fragment-Based Quantum Chemistry*

45. Intermolecular Interactions and Properties of Gases, Liquids and Solids
    - University of Graz, Austria (July 2023)
    - *High-Fidelity Fragmentation Via High-Order Many-Body Expansions*

44. ACS National Meeting, COMP Division Symposium on "Quantum Mechanics"
    - Indianapolis, IN (March 2023)
    - *Kohn-Sham Methods for Core-Level Spectroscopy*

43. ACS National Meeting, PHYS Division Symposium on "The Synergy of Theory and Experiment: A Symposium in Honor of Prof. John F. Stanton"
    - San Diego, CA (March 2022)
    - *Quantitative Protocol for Aqueous-Phase Ionization Energies Affords Insight into Anion–Water Hydrogen Bonding at the Air–Water Interface*

42. International Chemical Congress of Pacific Basin Societies ("Pacifichem"), Symposium on "Computational Quantum Chemistry: Synergism Between Theory and Experiment" in Honor of Henry F. Schaefer III
    - virtual (December 2021)
    - *Combining Continuum Electrostatics with Quantum Chemistry to Simulate Liquid Microjet Photoelectron Spectroscopy*

41. International Chemical Congress of Pacific Basin Societies ("Pacifichem"), Symposium on "Chemical Concepts from Theory and Computation"
    - virtual (December 2021)
    - *Reinterpreting π-Stacking*

40. International Chemical Congress of Pacific Basin Societies ("PacificChem"), Symposium on "Enabling Transformative Computational Chemistry Models on Exascale Computers"
    - virtual (December 2021)
    - *Simple, Robust, and Efficient Fragmentation Methods for Quantum Chemistry*

39. ACS National Meeting, COMP Division, Symposium on "Quantum Mechanics"
    - virtual (April 2021)
    - *Simple, Robust, and Efficient Fragmentation Methods for Quantum Chemistry Based on the Many-Body Expansion*

38. 10th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP)
    - Tromsø, Norway (July 2019)
    - *New Developments in Fragment-Based Quantum Chemistry*

37. 9th Triennial Conference on Molecular Quantum Mechanics Conference (MQM)
    - Heidelberg, Germany (July 2019)
    - *New Developments in Fragment-Based Quantum Chemistry*

36. ACS National Meeting, COMP Division Symposium on "Quantum Chemistry"
    ◦ Philadelphia, PA (August 2016)
    ◦ *Energy Decomposition Analysis with a Well-Defined Charge-Transfer Term for Interpreting Intermolecular Interactions*

35. ACS National Meeting, PHYS Division Symposium on "Accurate Characterization of Noncovalent Interactions: From Small Molecules to Supramolecular Chemistry"
    ◦ New Orleans, LA (April 2013)
    ◦ *A Cubic-Scaling Method with Chemical Accuracy for Non-Covalent Interactions*

34. ACS National Meeting, PHYS Division Symposium on "Excited-State Dynamics: Theory and Experiment"
    ◦ Denver, CO (August 2011)
    ◦ *Polarizable QM/MM Simulations of the Aqueous Electron: Excited States and More*

33. ACS National Meeting, PHYS Division Symposium on "Infrared Spectroscopy of Gas and Condensed Phase Biomolecules"
    ◦ Anaheim, CA (March 2011)
    ◦ *Towards ab Initio Prediction of Transient IR Spectra for Nucleic Acid Systems: New Tools for Excited States in Complex Systems*

32. ACS National Meeting, COMP Division Symposium on "Colloids: Gels, Sols, and Emulsions. You Know... Goo"
    ◦ Boston, MA (August 2010)
    ◦ *The Role of Solvent Polarization in the Spectroscopy of $e^-(aq)$*

31. ACS National Meeting, COMP Division Symposium on "Quantum Mechanics"
    ◦ San Francisco, CA (March 2010)
    ◦ *Balanced Treatment of Charge-Transfer Excitations in TD-DFT Using Long-Range-Corrected Functionals*

30. 64th International Symposium on Molecular Spectroscopy
    ◦ Columbus, OH (June 2009)
    ◦ *Trouble with TDDFT: A Public Service Announcement about Large-Scale Excited-State Calculations, with Application to DNA Oligomers*

29. Central Regional ACS Meeting
    ◦ Cleveland, OH (May 2009)
    ◦ *Attacking the Excited States of DNA with Some New Quantum Chemistry Tools*

28. ACS National Meeting, PHYS Division Symposium on "Progress in Polarizable Force Fields and Simulation"
    ◦ Salt Lake City, UT (March 2009)
    ◦ *An Electron–Water Pseudopotential for QM/MM Simulations of $(H_2O)_N^-$, from* $N = 2$ *to* $N = \infty$

27. ACS National Meeting, PHYS Division Symposium on "Computational Spectroscopy"
    ◦ New Orleans, LA (April 2008)
    ◦ *Excited Electronic States of Nucleic Acid Assemblies*

26. Midwest Theoretical Chemistry Conference
    ◦ Bloomington, IN (June 2007)
    ◦ *Quantum-Chemical Studies of the Structure and Spectroscopy of Solvated-Electron Clusters, $(H_2O)_n^-$ and $(HF)_n^-$*

25. 62nd International Symposium on Molecular Spectroscopy
    ◦ Columbus, OH (June 2007)

- *Spurious Charge-Transfer Contamination in Large-Scale TDDFT Calculations: A Public Service Announcement*

24. 62nd International Symposium on Molecular Spectroscopy
    - Columbus, OH (June 2007)
    - *First-Principles Quantum-Chemical Simulations of the Hydrated Electron, $(H_2O)_n^-$*

23. 61st International Symposium on Molecular Spectroscopy
    - Columbus, OH (June 2006)
    - *Anion–Water vs. Electron–Water Hydrogen Bonds*

22. 61st International Symposium on Molecular Spectroscopy
    - Columbus, OH (June 2006)
    - *$(H_2O)_n^-$ Photoelectron Spectra from ab Initio Molecular Dynamics Simulations*

21. Midwest Theoretical Chemistry Conference
    - Columbus, OH (June 2006)
    - *Anion–Water vs. Electron–Water Hydrogen Bonds*

20. Berkeley Chemical Dynamics Seminar
    - University of California, Berkeley, CA (October 2005)
    - *Structure, Electron Correlation, and Excess-Electron Dynamics in $(H_2O)_n^-$ Cluster Anions*

19. ACS National Meeting, PHYS Division Symposium on "Structures and Properties of Small Clusters"
    - Washington, DC (August 2005)
    - *Dynamics of the "Excess" Electron in Small Water Cluster Anions*

18. ACS National Meeting, PHYS Division Symposium on "Computational Exploration of Energy Landscapes."
    - Washington, DC (August 2005)
    - *Fast Algorithms for ab Initio Molecular Dynamics*

17. XXth Conference on the Dynamics of Molecular Collisions (DMC)
    - Pacific Grove, CA (July 2005)
    - *Structure and Dynamics of Water Cluster Anions, $(H_2O)_n^-$*

16. 60th International Symposium on Molecular Spectroscopy
    - Columbus, OH (June 2005)
    - *Inherent Structure and Excess Electron Dynamics of Water Cluster Anions, $(H_2O)_n^-$*

15. 60th International Symposium on Molecular Spectroscopy
    - Columbus, OH (June 2005)
    - *Fast Algorithms for ab Initio Molecular Dynamics*

14. Berkeley Radicals Seminar
    - University of California, Berkeley, CA (March 2005)
    - *Dynamical versus Electronic Control in the FONO $\rightarrow$ FNO_2 Isomerization Reaction*

13. Gordon Research Conference on Molecular Energy Transfer
    - Santa Barbara, CA (January 2005)
    - *FO + NO $\rightarrow$ FONO $\rightarrow$ FNO_2: Dynamic versus Electronic Control of a Unimolecular Isomerization Reaction*

12. Gordon Research Symposium on Molecular Energy Transfer
    - Santa Barbara, CA (January 2005)
    - *(Fictitious) Nuclear–Electron Energy Transfer in Car-Parrinello Molecular Dynamics*

11. ACS National Meeting, PHYS Division Symposium on "Physical Chemistry of the Atmosphere."
    - Philadelphia, PA (August 2004)
    - *Organonitrate Formation in the Atmosphere: A Unimolecular Mechanism for Pernitrite Isomerization, ROONO → $RONO_2$*

10. 59th International Symposium on Molecular Spectroscopy
    - Columbus, OH (June 2004)
    - *Nonadiabatic Dynamics of FO + NO: A Plausible Mechanism for Atmospheric $RONO_2$ Formation*

9. APS National Meeting
    - Montreal, Quebec (March 2004)
    - *Nonadiabatic Dynamics of FO + NO: Implications for Alkylpernitrite (ROO–N=O) Decomposition Pathways*

8. ACS National Meeting
    - New York, NY (August 2003)
    - *Toward a (One-Electron) Density Matrix Functional Theory*

7. XIXth Conference on the Dynamics of Molecular Collisions (DMC)
    - Tahoe, CA (July 2003)
    - *Density Matrix Functional Theory (DMFT): Non-Dynamical Correlation within a One-Electron Theory*

6. XIXth Conference on the Dynamics of Molecular Collisions (DMC)
    - Tahoe, CA (July 2003)
    - *Nonadiabatic Quantum Dynamics of the Reaction FO + NO → [FONO]* → F + NO_2*

5. Midwest Theoretical Chemistry Conference
    - Ames, IA (June 2003)
    - *Toward a One-Electron Density Matrix Functional Theory*

4. Great Lakes Regional ACS Meeting, Symposium in honor of John Pople
    - Chicago, IL (June 2003)
    - *A Reconstructive, Density-Matrix Approach to Natural Orbital Functional Theory*

3. 43rd Sanibel Symposium
    - St. Simons Island, GA (February 2003)
    - *N-Representability and Variational Stability in Natural Orbital (Density Matrix) Functional Theory*

2. American Mathematical Society Regional Meeting
    - Topeka, KS (April 1997)
    - *Cooperation and Conflict with Imperfect Communication: Prisoner's Dilemma with Noise*

1. American Mathematical Society Regional Meeting
    - McPherson, KS (April 1996)
    - *Cooperation and Conflict with Imperfect Communication: Prisoner's Dilemma with Noise*

Theses Supervised

20. Paige Bowling (Ph.D., 2024). Quantum Mechanical Approaches for Large Protein Systems: Fragmentation, Confining Potentials, and Anisotropic Solvation.

19. Suranjan Paul (Ph.D., 2022). Applications and Development of Generalized Dielectric Boundary Conditions to Solvated Systems in Bulk Water and Air/Water Interface.

18. Bhaskar Rana (Ph.D., 2021). Computational Spectroscopy and Molecular Dynamics Studies of Condensed-Phase Radicals Using Density Functional Theory.

17. Bushra Alam (Ph.D., 2021). Quantum Chemical Studies of Charge-Separated States and X-Ray Absorption Spectroscopy with Time Dependent Kohn-Sham Theory.

16. Kevin Carter-Fenk (Ph.D., 2021). Design and Implementation of Quantum Chemistry Methods for the Condensed Phase: Noncovalent Interactions at the Nanoscale and Excited States in Bulk Solution.

15. Ying Zhu (Ph.D., 2020). Implementation of Real-Time Time-Dependent Density Functional Theory and Applications from the Weak Field to the Strong Field Regime.

14. Saswata Dasgupta (Ph.D., 2020). *Ab-Initio* Implementation of Ground and Excited State Resonance Raman Spectroscopy: Application to Condensed Phase and Progress Towards Biomolecules.

13. Kuan-Yu Liu (Ph.D., 2019). Generalized Many-Body Expansion: A Fragment-Based Method for Modeling Large Systems.

12. Adrian F. Morrison (Ph.D., 2017). An Efficient Method for Computing Excited State Properties of Extended Molecular Aggregates Based on an *ab-Initio* Exciton Model.

11. Marc P. Coons (Ph.D., 2017). Solvent Effects for Vertical Ionization Processes in Liquid Water and at the Liquid-Vapor Interface.

10. Ying Zhu (M.S., 2016). A Comparison of Calculation by Real-Time and by Linear-Response Time-Dependent Density Functional Theory in the Regime of Linear Optical Response.

9. Xing Zhang (Ph.D., 2016). Spin-Flip Time-Dependent Density Functional Theory and its Applications to Photodynamics.

8. Ka Un Lao (Ph.D., 2016). Accurate and Efficient Quantum Chemistry Calculations for Noncovalent Interactions in Many-Body Systems.

7. Zachary C. Holden (Ph.D., 2015). Long-Range Effects in QM/MM Calculations: Ewald Summation in Non-Minimal Basis Sets.

6. Ryan M. Richard (Ph.D., 2013). Increasing the Computational Efficiency of *ab Initio* Methods with Generalized Many-Body Expansions.

5. Zachary C. Holden (M.S., 2012). The Theory of Ewald Summation Applied to QM/MM Systems.

4. Adrian W. Lange (Ph.D., 2012). Multi-Layer Methods for Quantum Chemistry in the Condensed Phase: Combining Density Functional Theory, Molecular Mechanics, and Continuum Solvation Models.

3. Leif D. Jacobson (Ph.D., 2011). Approximating Many-Body Induction to Efficiently Describe Molecular Liquids and Clusters with Improved Accuracy.

2. Ryan M. Richard (M.S., 2011). Time-Dependent Density-Functional Description of the ^1L_a State in Polycyclic Aromatic Hydrocarbons.

1. Shoumik Chatterjee (M.S., 2008). Charge Transfer States is Bianthyrl and Cyclophanes When Calculated with Conventional TD-DFT and with a Long-Range-Corrected Functional.

Courses Taught

- General Chemistry I (undergrad)
- Honors General Chemistry I (undergrad)
- Physical Chemistry I (undergrad quantum mechanics and spectroscopy)
- Physical Chemistry II (undergrad thermodynamics and statistical mechanics)
- Physical Chemistry III (undergrad chemical equilibria and kinetics)
- Quantum Chemistry I (graduate)
- Quantum Mechanics & Spectroscopy (graduate)
- Introduction to Electronic Structure Theory (graduate)
- Statistical Thermodynamics (graduate)
- Advanced Quantum Mechanics (graduate)

Service

- Chair-Elect, ACS Computers & Chemistry (COMP) Division (2025–)
- Chair, faculty search committee, "Theoretical Chemistry" (2024–2025)
- Programming Board, ACS Computers & Chemistry (COMP) Division (2023–2025)
- Director, NSF REU Site ("Experimental and Computational Spectroscopy"), 2022–
- Faulty search committee, Timashev Chair in Chemical Physics (2023–2024)
- Chair, faulty search committee, "Experimental Physical Chemistry" (2022–2023)
- Co-organizer, Midwest Theoretical Chemistry Conference (MWTCC) @ Ohio State (2022)
- Co-organizer (with M. Caricato), National ACS PHYS Division Symposium on "New Developments in Hybrid QM/QM, QM/MM, and Fragmentation Methods" (2022)
- Graduate Enrichment Committee, Ohio State University (2021)
- Promotion & Tenure Review Panel, Natural and Mathematical Sciences, Ohio State University (2019–)
- Organizer, Midwest Undergraduate Computational Chemistry Consortium (MU3C) Conference @ Ohio State, 2019.
- Editorial Board, Physical Chemistry Section, *Molecules* (2018–2021)
- Faculty Advisor, Ohio State chapter of oSTEM (2018–2023)
- Ohio State University Research Computing Committee (2018–2019)
- Chair, Ohio Supercomputer Center Statewide Users' Group (2017–)
- Physical Chemistry Division Secretary, Ohio State University (2016–)
- Chair, faculty search committee, "Theoretical Chemistry" (2016–2017)
- Organizer, Q-Chem Developers' Meeting, Philadelphia, PA (August 2016)
- International Scientific Advisory Committee, 10th International Conference on Computational Physics (2016–2017)
- Co-organizer (with M. Head-Gordon), National ACS PHYS Division Symposium on "Electronic Structure Theory for Large Systems", Boston, MA (August 2015)
- Editorial Advisory Board, *Journal of Physical Chemistry* (2014–2015)
- Chair, faculty search committee, "Data Analytics" (2014–2015)

- Chair, faculty search committee, "Experimental Molecular Biophysics" (2012–2013)
- Board of Directors for Q-Chem, Inc. (2012–)
- Vice Chair, Ohio Supercomputer Center Statewide Users' Group (2012–2014)
- Resource Allocation Committee for XSEDE (Extreme Science and Engineering Discovery Environment, formerly known as the NSF TeraGrid), 2011–2017. (≈ 50 proposals to review per year.)
- Co-organizer (with S. Bradforth), National ACS PHYS Division Symposium on "Excited-State Dynamics: Theory and Experiment", Denver, CO (September 2011)
- Organizer, Central Regional ACS Symposium on "Theoretical Modeling of Solvation: Methods and Applications", Columbus, OH (June 2008)
- Faculty Advisor, OSU Physical Chemistry Student Lecture Series (2007–2015)
- Organizer, OSU Physical Chemistry Seminar (2006–2013)

Funding

- *Multiscale Methods for Electronic Structure Theory*
  Dept. of Energy, Office of Basic Energy Sciences, $550,000 (2025–2027).
- *Wavefunction Embedding: A Toolbox for Transition Metal Spectroscopy*
  National Science Foundation, Chemistry Division, $508,776 (2024–2027).
- *Quantum Chemistry Methods for Rational Drug Design*
  National Institutes of Health, $247,909 (2023–2024). (SBIR with Q-Chem, Ohio State sub-award: $80,000.)
- *REU Site: Experimental and Computational Spectroscopy: Fundamental Probes of Molecules, Molecular Interactions, and Materials*
  National Science Foundation, Chemistry Division, $388,369 (2022–2025).
- *High-Fidelity Fragment-Based Quantum Chemistry for Macromolecules, Condensed Phases, and Complex Environments*
  Dept. of Energy, Office of Basic Energy Sciences, $507,466 (2020–2024).
- *Fundamental Theoretical Studies of the Redox Properties of Catalytic Metal Oxide Nanoparticles*
  American Chemical Society Petroleum Research Fund, $110,000 (2021–2023).
- *Quantum Chemistry Methods for Excited States at Liquid- and Solid-State Interfaces*
  National Science Foundation, Chemistry Division, $507,466 (2020–2024).
- *Quantum Simulations of Electron Dynamics in Aqueous Systems*
  National Science Foundation, Chemistry Division, $450,000 (2017–2021).
- *Fragment-Based Quantum Chemistry for Intermolecular Interactions and Exciton Transport in Molecular Liquids and Solids*
  Dept. of Energy, Office of Basic Energy Sciences, $428,628 (2017–2020).
- *New Methods for Describing Electronic Excitation, Ionization, and Electrostatics of Complex Systems in Aqueous Environments*
  National Science Foundation, Chemistry Division, $442,059 (2014–2017).
- *Development of Accurate and Affordable Electronic Structure Methods for the Condensed Phase*
  Dept. of Energy, Office of Basic Energy Sciences. $430,721 (2012–2016).
- Camille Dreyfus Teacher-Scholar Award. $75,000 (2011–2016)
- Alfred P. Sloan Foundation Research Fellowship. $50,000 (2010–2014).
- *Characterizing Excited Electronic States of DNA Using Novel Methods Based on Time-Dependent Density-Functional Theory*

National Science Foundation CAREER Award, Chemistry Division, $625,000 (2008–2012).

- Ab initio *Molecular Dynamics and* ab Initio *Quantum Dynamics Investigation of Radical Reactions Involved in Combustion*
  ACS Petroleum Research Fund (Type G Grant). $40,000 (2007–2009).