Contact Information

Department of Chemistry & Biochemistry
The Ohio State University
100 W. 18th Ave.
Columbus, OH 43210

Voice: (614) 292-6851
Fax: (614) 292-1685
herbert@chemistry.ohio-state.edu
www.chemistry.ohio-state.edu/~herbert

Employment

- Professor, The Ohio State University (2014–present)
- Associate Professor, The Ohio State University (2011–2014)
- Assistant Professor, The Ohio State University (2006–2011)

Education

- Ph.D., Physical Chemistry
  University of Wisconsin, Madison, WI (August 1999–May 2003)
- B.Sc., Mathematics & Chemistry
  Kansas State University, Manhattan, KS (August 1994–December 1998)

Selected Awards

- Edward W. Morley Medal, American Chemical Society, 2020
- Alexander von Humboldt Foundation Fellowship, 2016–2019
- 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 Mathematical Sciences Postdoctoral Fellowship, 2004–2006
- National Defense Science & Engineering Graduate Fellowship (NDSEG), 1999–2002
- NSF Pre-Doctoral Fellowship, 1999 (declined in favor of NDSEG award)

Most Cited Publications

Out of 121 total publications (9,621 total citations); h-index = 44 (Google Scholar).

92. J. M. Herbert and M. P. Coons. The hydrated electron. *Annu. Rev. Phys. Chem.* **68**, 447 (2017). **[67 citations]**

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). **[51 citations]**

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). **[55 citations]**

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). **[49 citations]**

73. K. U. Lao, R. Schäffer, G. Jansen, and J. M. Herbert. Accurate description of intermolecular interactions involving ions using symmetry-adapted perturbation theory. *J. Chem. Theory Comput.* **11**, 2473 (2015). **[57 citations]**

72. J.-M. Mewes, Z.-Q. You, M. Wormit, T. Kriesche, J. M. Herbert, and A. Dreuw. Experimental benchmark data and systematic evaluation of two *a posteriori*, polarizable-continuum corrections for vertical excitation energies in solution. *J. Phys. Chem. A* **119**, 5446 (2015). **[87 citations]**

69. K. U. Lao and J. M. Herbert. Accurate and efficient quantum chemistry calculations of noncovalent interactions in many-body systems: The XSAPT family of methods. *J. Phys. Chem. A* **119**, 235 (2015). **[63 citations]**

68. Y. Shao *et al.* Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Mol. Phys.* **113**, 184 (2015). **[1,768 citations]**

66. R. M. Richard, K. U. Lao, and J. M. Herbert. Aiming for benchmark accuracy with the many-body expansion. *Acc. Chem. Res.* **47**, 2828 (2014). **[63 citations]**

64. X. Zhang and J. M. Herbert. Analytic derivative couplings for spin-flip configuration interaction singles and

spin-flip time-dependent density functional theory. *J. Chem. Phys.* **141**, 064104 (2014). **[66 citations]**

62. R. M. Richard, K. U. Lao, and J. M. Herbert. Understanding the many-body expansion for large systems. I. Precision considerations. *J. Chem. Phys.* **141**, 014108 (2014). **[51 citations]**

56. K. U. Lao and J. M. Herbert. An improved treatment of empirical dispersion and a many-body energy decomposition scheme for the explicit polarization plus symmetry-adapted perturbation theory (XSAPT) method. *J. Chem. Phys.* **139**, 034107 (2013). **[59 citations]**

52. R. M. Richard and J. M. Herbert. A generalized many-body expansion and a unified view of fragment-based methods in electronic structure theory. *J. Chem. Phys.* **137**, 064113 (2012). **[148 citations]**

50. J. M. Herbert, L. D. Jacobson, K. U. Lao, and M. A. Rohrdanz. Rapid computation of intermolecular interactions in molecular and ionic clusters: Self-consistent polarization plus symmetry-adapted perturbation theory. *Phys. Chem. Chem. Phys.* **14**, 7679 (2012). **[51 citations]**

48. J. M. Herbert and L. D. Jacobson. Structure of the aqueous electron: Assessment of one-electron pseudopotential models in comparison to experimental data and time-dependent density functional theory. *J. Phys. Chem. A* **115**, 14470 (2011). **[61 citations]**

45. A. W. Lange and J. M. Herbert. Symmetric versus asymmetric discretization of the integral equations in polarizable continuum solvation models. *Chem. Phys. Lett.* **509**, 77 (2011). **[57 citations]**

43. R. M. Richard and J. M. Herbert. Time-dependent density-functional description of the ^1L_a state in polycyclic aromatic hydrocarbons: Charge-transfer character in disguise?. *J. Chem. Theory Comput.* **7**, 1296 (2011). **[135 citations]**

42. L. D. Jacobson and J. M. Herbert. Comment on "Does the hydrated electron occupy a cavity?". *Science* **331**, 1387 (2011). **[95 citations]**

40. L. D. Jacobson and J. M. Herbert. An efficient, fragment-based electronic structure method for molecular systems: Self-consistent polarization with perturbative two-body exchange and dispersion. *J. Chem. Phys.* **134**, 094118 (2011). **[78 citations]**

39. J. M. Herbert and L. D. Jacobson. Nature's most squishy ion: The important role of solvent polarization in the description of the hydrated electron. *Int. Rev. Phys. Chem.* **30**, 1 (2011). **[51 citations]**

38. A. W. Lange and J. M. Herbert. A smooth, nonsingular, and faithful discretization scheme for polarizable continuum models: The switching/Gaussian approach. *J. Chem. Phys.* **133**, 244111 (2010). **[108 citations]**

37. D. Ghosh, D. Kosenkov, V. Vanovschi, C. F. Williams, J. M. Herbert, M. S Gordon, M. W. Schmidt, L. V. Slipchenko, and A. I. Krylov. Noncovalent interactions in extended systems described by the effective fragment potential method: Theory and applications to nucleobase oligomers. *J. Phys. Chem. A* **114**, 12739 (2010). **[118 citations]**

36. L. D. Jacobson and J. M. Herbert. A one-electron model for the aqueous electron that includes many-body electron–water polarization: Bulk equilibrium structure, vertical electron binding energy, and optical absorption spectrum. *J. Chem. Phys.* **133**, 154506 (2010). **[74 citations]**

34. A. W. Lange and J. M. Herbert. Polarizable continuum reaction-field solvation models affording smooth potential energy surfaces. *J. Phys. Chem. Lett.* **1**, 556 (2010). **[86 citations]**

32. L. D. Jacobson, C. F. Williams, and J. M. Herbert. The static-exchange electron–water pseudopotential, in conjunction with a polarizable water model: A new Hamiltonian for hydrated-electron simulations. *J. Chem. Phys.* **130**, 124115 (2009). **[56 citations]**

31. A. W. Lange and J. M. Herbert. Both intra- and interstrand charge-transfer excited states in aqueous B-DNA are present at energies comparable to, or just above, the $^1\pi\pi^*$ excitonic bright states. *J. Am. Chem. Soc.* **131**, 3913 (2009). **[184 citations]**

30. M. A. Rohrdanz, K. M. Martins, and J. M. Herbert. A long-range-corrected density functional that performs well for both ground-state properties and time-dependent density functional theory excitation energies, including charge-transfer excited states. *J. Chem. Phys.* **130**, 054112 (2009). **[500 citations]**

29. M. A. Rohrdanz and J. M. Herbert. Simultaneous benchmarking of ground- and excited-state properties with long-range-corrected density functional theory. *J. Chem. Phys.* **129**, 034107 (2008). **[274 citations]**

27. A. W. Lange, M. A. Rohrdanz, and J. M. Herbert. Charge-transfer excited states in a π-stacked adenine dimer, as predicted using long-range-corrected time-dependent density functional theory. *J. Phys. Chem. B* **112**, 6304 (2008). **[166 citations]**

26. P. M. Hare, C. T. Middleton, K. I. Mertel, J. M. Herbert, and B. Kohler. Time-resolved infrared spectroscopy of the lowest triplet state of thymine and thymidine. *Chem. Phys.* **347**, 383 (2008). **[63 citations]**

25. A. Lange and J. M. Herbert. Simple methods to reduce charge-transfer contamination in time-dependent density-functional calculations of clusters and liquids. *J. Chem. Theory Comput.* **3**, 1680 (2007). **[90 citations]**

21. J. M. Herbert and M. Head-Gordon. Charge penetration and the origin of large vibrational red-shifts in hydrated-electron clusters, $(H_2O)_n^-$. *J. Am. Chem. Soc.* **128**, 13932 (2006). **[61 citations]**

20. J. M. Herbert and M. Head-Gordon. First-principles, quantum-mechanical simulation of electron solvation by a water cluster. *Proc. Natl. Acad. Sci. USA* **103**, 14282 (2006). **[68 citations]**

19. Y. Shao *et al*. Advances in methods and algorithms in a modern quantum chemistry program package. *Phys. Chem. Chem. Phys.* **8**, 3172 (2006). **[2,546 citations]**

18. J. M. Herbert and M. Head-Gordon. Accuracy and limitations of second-order many-body perturbation theory for predicting vertical detachment energies of solvated-electron clusters. *Phys. Chem. Chem. Phys.* **8**, 68 (2006). **[91 citations]**

16. J. M. Herbert and M. Head-Gordon. Accelerated, energy-conserving Born-Oppenheimer molecular dynamics *via* Fock matrix extrapolation. *Phys. Chem. Chem. Phys.* **7**, 3269 (2005). **[99 citations]**

14. J. M. Herbert and M. Head-Gordon. Calculation of electron detachment energies for water cluster anions: An appraisal of electronic structure methods, with application to $(H_2O)_{20}^-$ and $(H_2O)_{24}^-$. *J. Phys. Chem. A* **109**, 5217 (2005). **[140 citations]**

13. J. M. Herbert and M. Head-Gordon. Curvy-steps approach to constraint-free extended-Lagrangian molecular dynamics, using atom-centered basis functions: Convergence toward Born–Oppenheimer trajectories. *J. Chem. Phys.* **121**, 11542 (2004). **[70 citations]**

10. J. M. Herbert and J. E. Harriman. *N*-representability and variational stability in natural orbital functional theory. *J. Chem. Phys.* **118**, 10835 (2003). **[60 citations]**

Presentations

- 54 department seminars (19 international)
- 99 invited conference presentations (20 international)
- 30 contributed conference presentations (3 international)

Theses Supervised

- 11 Ph.D. & 3 M.S. completed
- 9 current Ph.D. students

Selected Service

- Co-organizer, Midwest Theoretical Chemistry Conference (MWTCC) @ Ohio State, 2021.
- Organizer, Midwest Undergraduate Computational Chemistry Consortium (MU3C) Conference @ Ohio State, 2019.
- Editorial Board (Physical Chemistry Section), *Molecules* (2018–)
- Chair, Ohio Supercomputer Center Statewide Users' Group, 2017–
- Chair, faculty search committees in 2012, 2014, & 2016
- Co-organizer (with M. Head-Gordon), National ACS PHYS Division Symposium "Electronic Structure Theory for Large Systems" (2015) and (with S. Bradforth) "Excited-State Dynamics: Theory and Experiment" (2011).
- Editorial Advisory Board, *Journal of Physical Chemistry* (2014–2015)
- 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.

Current Funding

1. Fundamental theoretical studies of the redox properties of catalytic metal oxide nanoparticles. American Chemical Society Petroleum Research Fund, $110,00 (2021–2023).
2. High-fidelity fragment-based quantum chemistry for macromolecules, condensed phases, and complex environments. Dept. of Energy, Office of Basic Energy Sciences, $507,466 (2020–2023).
3. Quantum chemistry methods for excited states at liquid- and solid-state interfaces. National Science Foundation, $507,466 (2020–2023).
4. Quantum simulations of electron dynamics in aqueous systems. National Science Foundation, $450,000 (2017–2021).