Curriculum Vitae
William James Glover

Contact Information
NYU Shanghai
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Online profiles
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Google Scholar: https://scholar.google.com/citations?user=bBcKFxwAAAAJ&hl=en

Titles and Affiliations

NYU Shanghai, China

2024/09 –	Associate Professor of Chemistry
2015/09 – 2024/09	Assistant Professor of Chemistry
2022/09 – Present	Graduate Coordinator of Chemistry

NYU-ECNU Center for Computational Chemistry, Shanghai, China

2024/09 –	Director
2019/03 – 2024/09	Associate Director
2015/09 – Present	Faculty Member

Shanghai Frontiers Science Center of Artificial Intelligence and Deep Learning, China

2023/03 – Present	Faculty Member

Department of Chemistry, New York University, NY, USA

2024/09 –	Global Network University Associate Professor of Chemistry
2015/09 – 2024/09	Global Network University Assistant Professor of Chemistry

Professional Preparation

1999/10 – 2003/06	MChem, Oxford University, 1st-class honors (summa cum laude) 2nd August 2003 (Advisor: Prof. Paul A. Madden)
2003/09 – 2009/12	Ph.D, Physical chemistry, University of California, Los Angeles, 11th December 2009 (Advisor: Prof. Benjamin J. Schwartz)
2010/02 – 2013/02	Postdoctoral Fellow, Stanford University (Advisor: Prof. Todd J. Martinez)
2013/02 – 2015/09	Postdoctoral Scholar, University of California, Los Angeles (Advisor: Prof. Benjamin J. Schwartz)

Awards

2024/5/9	NYU Shanghai Teaching Excellence Award AY 23-24 (awarded to 3 faculty)
2023/12/01	2023 Pudong Pearl Talents Program (Leading Scheme)
2023/03/29	Spring 2023 ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry

Grants

Awarded as Principal Investigator:

2022/01 MOST Foreign Young Talents Program. 2 years.
2022/01 NSFC Research Fund for International Excellent Young Scientists. 2 years.
2022/01 NSFC General Grant. 4 years.
2021/01 MOST National Foreign Experts Program Fund. 2 years.
2021/01 STCSM Foreign Experts Program. 1 year.
2019/01 NSFC Research Fund for International Young Scientists. 1 year.
2018/01 NSFC Research Fund for International Young Scientists. 1 year.
2017/01 Natural Science Foundation of China, Young Scientists Fund. 3 years.

Awarded as Co-Principal Investigator:

2017/03 NYU-ECNU Joint Research Institute Seed Grant for Collaborative Research with Xiao He (ECNU, China). 2 years.

2016/02 NYU Global Seed Grant for Collaborative Research with John Z. H. Zhang (NYUSH), and Yingkai Zhang (NYU). 2 years.

Awarded as Participant:

2023/03 "Frontier Scientific Research Center for Artificial Intelligence and Deep Learning". Shanghai Municipal Education Commission. PI/Director: Keith Ross. Participants: Bruno Abrahao, Tim Byrnes, Yuxin Chen, Zhibin Chen, William Glover, Li Guo, Siyao Guo, Xin Jin, Mathieu Laurière, Li Li, Sukbin Lim, Shuyang Ling, Guyue Liu, Yik-Cheung Tam, Xing Tian, Dan Wang, Shengjie Wang, Hongyi Wen, Gus Xia, Jie Xue, and John Zhang. 3 years.

2018/04 NSFC-RS International Cooperation and Exchange Program, awarded unilaterally by Royal Society. PI: Jan R. R. Verlet (Durham, UK). 2 years.

Teaching experience

Courses developed:

Fall 19: Computational Chemistry (Graduate level course in Quantum Chemistry, Molecular Modelling, Molecular Dynamics)
Spring 18: Computational Chemistry (Undergraduate introductory course in Quantum Chemistry, Molecular Modelling, Molecular Dynamics)

Courses taught:

Spr. 21,22: Graduate Computational Chemistry
Fall 19: Graduate Computational Chemistry
Spr. 18,19: Computational Chemistry
Fall 16-18,22,23: Foundations of Chemistry I (General Chemistry topics including Atomic Theory, Chemical Structure, Thermodynamics, Quantum Mechanics, and Molecular Orbital Theory)
Spr. 17, 23,24: Foundations of Chemistry II (General Chemistry topics including Intermolecular Forces, Kinetics, Crystal Structure, Transition Metals, and Chemical Equilibria)

Student mentoring

Masters and Doctoral Dissertation Committee

2023/09 – Yuzhi Xu (John Zhang Group, NYUSH)
2023/06 – 2024/05 Kai Chen (William Glover Group, NYUSH)
2022/11 – Fanyu Zhao (John Zhang Group, NYUSH)
2021/11 – Muchen Tong (Mark Tuckerman Group, NYUNY)
2021/10 – Shiyu Hu (John Zhang Group, NYUSH)
2021/10 – 2022/12 Dominikus Brian (M.S., Xiang Sun Group, NYUSH)
2021/06 – Yuquan Cao (William Glover Group, NYUSH)

2020/09 – 2022/06 Marek Narozniak (PhD, Tim Byrnes Group, NYUSH)
2019/09 – 2023/01 Amiel Paz (PhD, William Glover Group, NYUSH). Now Postdoc fellow at Stanford.
2018/09 – 2023/09 Yuanming Bai (PhD, William Glover Group, NYUSH). Now Research Scientist at Solvay.
2018/09 – 2023/05 Xingpin Li (PhD, William Glover Group, NYUSH). Now Olympiad Coach, Xishan highschool
2017/09 – 2021/09 Camille Farfan (PhD, Daniel Turner Group, NYU NY)

Undergraduate Thesis/Capstone Advisor
2023/09 – 2024/05 Yu Shen. Now PhD student in Chemistry at NYU Abu Dhabi.
2020/09 – 2020/12 Shaoting Peng. Now PhD student in Chemistry at NYU Abu Dhabi.
2018/09 – 2019/05 Jade Basinski. Now PhD student in Environmental Science at Northwestern.

Independent Studies
2017/09 – 2017/12 Omer Cohen. Now PhD student at Weizmann.
2017/09 – 2018/05 Qingchuan Sang. Now PhD student at Vanderbilt.

Deans Undergraduate Research Fund Advisor
2023/06 – 2023/08 Jiesong Lan. Current NYU Shanghai undergraduate Chemistry major.
2019/06 – 2019/09 Shaoting Peng. Now PhD student at NYU Abu Dhabi.
2018/06 – 2018/09 Hengyuan (Steve) Shen. Now PhD student in Chemistry at UC Berkeley.

Conferences organized
2024/06/29 2024 International Symposium on Computational Molecular Science and Machine Learning, Shanghai, China
2019/06/01 International Symposium on Quantum Effects in Chemistry and Biology, Shanghai, China
2016/07/23 International Workshop on Frontiers in Molecular Biophysics, Shanghai, China

Symposia organized
2024/03/04 "Machine Learning for Electronic Structures, Properties and Dynamics of Molecules and Materials". APS March Meeting, Minneapolis, USA

Service
University Administration
2022/09 – Graduate Coordinator for Chemistry, NYU Shanghai
2019/03 – Associate Director of NYU-ECNU Center for Computational Chemistry at NYU Shanghai
2018/09 – 2019/08 Graduate Coordinator for Chemistry, NYU Shanghai
2016/09 – 2019/08 Area Coordinator for Chemistry, NYU Shanghai [catch-all title encompassing duties of Department Chair & Director of Undergraduate Studies]

University Committee
2022/09 – Chair: HPC Committee, NYU Shanghai
2019/09 – 2021/09 Curriculum Committee, NYU Shanghai
2016/11 – 2019/06 Chair: Faculty Housing Committee, NYU Shanghai
2015/09 – 2016/09 Chair: Academic Technologies and Innovation Committee, NYU Shanghai

Journal
2005 – Reviewer for *Nature Comm.*, *J. Am. Chem. Soc.*, *J. Phys. Chem. Lett.*, *J. Phys. Chem.*, *J. Chem. Phys.*, *J. Chem. Theory Comput.*, *J. Chem. Inf. Model.*, *Chem. Phys. Lett.*, and *Phys. Chem. Chem. Phys.*

Conferences
2020, 2021 Referee for CECAM summer school in Quantum and Mixed Quantum Classical Dynamics in photochemistry

Publications and presentations as an independent researcher

Published or accepted in a peer-reviewed journal (indicates corresponding author)*

18. A. Humeniuk*, **WJG***, "Multistate, polarizable QM/MM embedding scheme based on the direct reaction field method: Solvatochromic shifts, analytical gradients and optimization of conical intersections in solution" *J. Chem. Theory Comp.* (2024). https://doi.org/10.1021/acs.jctc.3c01018

17. A. S. P. Paz, **WJG***, "Efficient analytical gradients of property-based diabatic states: Geometry optimizations for localized holes", *J. Chem. Phys.* **158**, 204107 (2023) https://doi.org/10.1063/5.0142590 [**Editors' Choice**][**Cover article**]

16. Y. Bai, L. Vogt-Maranto, M. E. Tuckerman, **WJG***, "Machine learning the Hohenberg-Kohn map to molecular excited states" ***Nat. Commun.*** **13**, 7044 (2022) https://doi.org/10.1038/s41467-022-34436-w [**Featured article**, **Press release**: https://shanghai.nyu.edu/news/scientists-develop-artificial-intelligence-predict-photochemical-reactions]

15. X. Li, X. Jia, A. S. P. Paz, Y. Cao, **WJG***, "Direct evidence for water antibonding orbital mixing in the hydrated electron from its X-ray absorption spectrum" ***J. Am. Chem. Soc.*** **144**, 19668-19672 (2022) https://doi.org/10.1021/jacs.2c07572 [**Press release**: https://shanghai.nyu.edu/news/new-nyu-shanghai-study-explores-nature-hydrated-electrons]

14. X. Liu, A. Humeniuk, **WJG***, "Conical intersections in solution with polarizable embedding: Integral-exact direct reaction field" *J. Chem. Theory Comput.* **18**, 6826-6839 (2022) https://doi.org/10.1021/acs.jctc.2c00662

13. A. Humeniuk*, **WJG***, "Efficient CPU and GPU implementations of multicenter integrals over long-range operators using Cartesian Gaussian functions", *Comput. Phys. Commun.* **280**, 108467 (2022) https://doi.org/10.1016/j.cpc.2022.108467

12. S. Karashima, A. Humeniuk, **WJG**, T. Suzuki*, "Ultrafast Photoisomerization of Ethylene Studied using Time-Resolved Extreme Ultraviolet Photoelectron Spectroscopy", *J. Phys. Chem. A* **126**, 3873-3879 (2022) https://doi.org/10.1021/acs.jpca.2c02468

11. Z. Shen, S. Peng, **WJG***, "Flexible boundary layer using exchange for embedding theories. II. QM/MM dynamics of the hydrated electron" *J. Chem. Phys.* **155**, 224113 (2021) https://doi.org/10.1063/5.0067861

10. Z. Shen, **WJG***, "Flexible boundary layer using exchange for embedding theories. I. Theory and implementation" *J. Chem. Phys.* **155**, 224112 (2021) https://doi.org/10.1063/5.0067855

9. A. S. P. Paz, N. S. Baleeva, **WJG***, "Active Orbital Preservation for Multiconfigurational Self-Consistent Field" *J. Chem. Phys.* **155**, 071103 (2021) https://doi.org/10.1063/5.0058673

8. C. Shen, X. Jin, **WJG**, X. He, "Accurate Prediction of Absorption Spectral Shifts of Proteorhodopsin Using a Fragment-based Quantum Mechanical Method" *Molecules* **26**, 4486 (2021) https://doi.org/10.3390/molecules26154486

7. A. S. P. Paz, **WJG***, "Diabatic Many-Body Expansion: Development and Application to Charge-Transfer Reactions" *J. Chem. Theory Comput.* **17**, 1497 (2021) https://doi.org/10.1021/acs.jctc.0c01231

6. B. F. E. Curchod, **WJG***, T. J. Martínez, "SSAIMS – Stochastic-Selection Ab Initio Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics", *J. Phys. Chem. A* **124**, 6133 (2020) https://doi.org/10.1021/acs.jpca.0c04113

5. X. Jin, **WJG*,** X. He*, "Fragment Quantum Mechanical Method for Excited-state Properties of the Green Fluorescent Protein" *J. Chem. Theory Comput.* **16**, 5174 (2020) https://doi.org/10.1021/acs.jctc.9b00980

4. **WJG*,** A. S. P. Paz, W. Thongyod, C. Punwong, "Analytical Gradients and Derivative Couplings for Dynamically Weighted Complete Active Space Self-Consistent Field" *J. Chem. Phys.* **151**, 201101 (2019) https://dx.doi.org/10.1063/1.5130997

3. J. Liu, H. Sun, **WJG**, X. He*, "Prediction of Excited-State Properties of Oligoacene Crystals Using Fragment-Based Quantum Mechanical Method" *J. Phys. Chem. A* **123**, 5407 (2019) https://dx.doi.org/10.1021/acs.jpca.8b12552

2. B. K. Petkov, T. A. Gellen, C. A. Farfan, W. P. Carbery, B. E. Hetzler, D. Trauner, X. Li, **WJG**, D. J. Ulness, D. B. Turner*, "Two-Dimensional Electronic Spectroscopy Reveals the Spectral Dynamics of Förster Resonance Energy Transfer", *Chem* **5**, 2111 (2019) https://dx.doi.org/10.1016/j.chempr.2019.05.005

1. M. A. Hagras and **WJG***, "Polarizable Embedding for Excited-State Reactions: Dynamically Weighted Polarizable QM/MM", *J. Chem. Theory Comput.* **14**, 2137 (2018) http://dx.doi.org/10.1021/acs.jctc.8b00064

Unpublished papers (indicates corresponding author)*

4. Y Bai, A. S. P. Paz, **WJG***, "UV photoresponse of the GFP chromophore in gas and aqueous phase: A simulation study" *To be submitted* (2023)

3. W. Thongyod, Y. Bai, C. Punwong, **WJG***, "UV response of the green fluorescent protein chromophore: Insights from ab initio non-adiabatic simulations" *To be submitted* (2023)

2. A. Humeniuk*, Y. Cao, A. S. P. Paz, **WJG***, "Role of electronic polarization in the primary charge-transfer states of the purple bacteria reaction center: A polarizable QM/MM study with the integral-exact direct reaction field method" *Under Revision* (2023). Pre-print: https://doi.org/10.26434/chemrxiv-2022-mkfzd

1. A. S. P. Paz, **WJG***, "Molecular origins of the ultrafast relaxation of a photoexcited hydrated electron" *Under Revision Following Review in* ***Science*** (2023). Pre-print: https://doi.org/10.26434/chemrxiv-2023-5kl9x

Invited talks

2024/10/13 11th Triennial Congress of the International Society for Theoretical Chemical Physics, Qingdao
2024/07/01 PhysChem24 and Hush Symposium, University of Sydney, Australia
2023/11/29 2nd International Symposium on Machine Learning in Quantum Chemistry, Uppsala, Sweden
2023/09/15 NYU, Chemistry Department Seminar, NY, USA
2023/09/14 Hebrew University Department of Chemistry Seminar, Jerusalem, Israel
2023/09/10 CECAM Multiscale Simulation of Photoresponsive Biological Systems, Tel Aviv, Israel
2023/06/29 2023 TDDFT Workshop: Excited states and dynamics, Rutgers University, New Jersey, USA
2023/06/19 UCL, Chemistry Department Seminar, London, UK
2023/06/14 Durham University, Chemistry Department Seminar, Durham, UK
2023/06/03 32nd Miller Conference on Radiation Chemistry, Furiani, Corsica Island, France
2023/05/12 Symposium on Computational Biology, Shandong University, Qingdao
2023/04/06 Harvard/MIT/Boston University Theoretical Chemistry Student Seminar Series, Boston, USA
2023/04/05 Stanford University, Chemistry Department Seminar, Stanford, USA
2023/03/26 American Chemical Society National meeting, Indianapolis
2023/03/06 University of Chicago, Chemistry Department Seminar (virtual)
2023/02/19 10th Asia-Pacific Association of Theoretical and Computational Chemists, Quy Nhon, Vietnam
2022/12/08 Duke University, Chemistry Department Seminar (virtual)
2022/11/29 University of Southern California, Chemistry Department Seminar (virtual)
2022/11/22 UC Riverside, Chemistry Department Seminar (virtual)
2022/11/02 Johns Hopkins University, Chemistry Department Seminar (virtual)
2022/10/28 University of Pennsylvania, Chemistry Department Seminar (virtual)
2022/10/27 Emory University, Chemistry Department Seminar (virtual)
2022/10/25 Texas Tech, Chemistry Department Seminar (virtual)
2022/10/18 Bristol University, Computational Chemistry, Theory, and Dynamics theme Seminar (virtual)
2022/10/05 UC Davis Chemistry Department Seminar (virtual)
2022/10/04 UC Santa Cruz Chemistry & Biochemistry Department Seminar (virtual)
2022/09/28 Yale University, Theoretical Chemistry Division Seminar (virtual)

2022/09/17 University of Nevada, Reno, Chemistry Department Seminar (virtual)
2022/07/20 VISTA online seminar
2022/06/23 Stony Brooke University Institute for Advanced Computational Science Department Seminar (virtual)
2022/06/17 Kyoto University Chemistry Department Seminar (virtual)
2022/06/14 UW Madison, Institute of Theoretical Chemistry Department Seminar (virtual)
2022/06/10 Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems, Teluride, Colorado
2022/05/27 Chinese University of Hong Kong Chemistry Department Seminar (virtual)
2022/05/21 UC Merced Chemistry Department Seminar (virtual)
2022/03/20 American Chemical Society National meeting, San Diego (virtual session)
2019/12/6 The Eighth Cross-Strait Conference on Theoretical and Computational Chemistry, Taipei, Taiwan
2019/08/11 TDDFT – Excited States and Dynamics, Rutgers University, New Jersey
2019/06/01 International Symposium on Quantum Effects in Chemistry and Biology, NYU Shanghai
2018/11/12 Second Middle-Eastern Materials Science Conference, NYU Abu Dhabi
2018/08/04 First Conference of Theoretical and Computational Chemistry, Beijing National Laboratory for Molecular Sciences
2018/06/12 Computational Chemical Dynamics: A Symposium in Honor of Donald J. Kouri, NYU Shanghai
2018/06/05 International center of quantum and molecular structure, Shanghai University
2018/03/11 International Symposium on Frontiers in Chemical Biology, NYU Shanghai
2017/11/01 STEM seminar series, NYU Shanghai
2017/10/27 Theoretical Chemistry Department Seminar, Beijing Normal University
2017/10/26 Theoretical Chemistry Department Seminar, Peking University
2016/11/16 STEM seminar series, NYU Shanghai
2016/07/23 Frontiers in Computational Chemistry International Workshop, NYU Shanghai
2016/07/04 Chinese Chemical Society Annual Meeting, Dalian
2016/05/26 Sino-German Workshop on Biomolecular Simulations Across Scales, Shanghai
2016/01/13 NYU-ECNU Center for Computational Chemistry at NYU Shanghai, Shanghai

Contributed talks
2024/03/04 American Physical Society Annual Meeting, Minneapolis, USA
2023/06/26 2023 ICQC Congress, Bratislava, Slovakia
2022/08/25 American Chemical Society National meeting, Chicago (Virtual session)
2021/08/22 American Chemical Society National meeting, Atlanta (Virtual session)
2021/05/03 Les Houches Workshop on Quantum Dynamics & Spectroscopy, Virtual
2019/11/18 The 2nd Quantum International Frontiers, Shanghai University, China
2019/09/30 Asia-Pacific Association of Theoretical and Computational Chemists, Sydney, Australia
2019/08/25 American Chemical Society National meeting, San Diego
2018/08/21 American Chemical Society National meeting, Boston
2017/08/27 WATOC 2017, Munich, Germany
2017/08/21 National Conference on Chemical Dynamics, Nanjing
2017/06/08 National Conference on Quantum Chemistry, Dalian
2016/10/25 International Conference on Molecular Simulation, Shanghai Jiao Tong University
2016/08/22 American Chemical Society National meeting, Philadelphia

<u>Publications and presentations before independent career</u>
Published or accepted in a peer-reviewed journal (indicates corresponding author)*
27. **WJG*,** B. J. Schwartz*, "The Fluxional Nature of the Hydrated Electron: Energy and Entropy Contributions to Aqueous Electron Free Energies" *J. Chem. Theory Comput.* **16**, 1263 (2020) https://doi.org/10.1021/acs.jctc.9b00496

26. **WJG,** T. Mori, M. S. Schuurman, A. E. Boguslavskiy, O. Schalk, A. Stolow, T. J. Martínez*, "Excited state non-

adiabatic dynamics of the smallest polyene, *trans* 1,3-butadiene. II. *Ab initio* multiple spawning simulations", *J. Chem. Phys.* **148**, 164303 (2018) https://doi.org/10.1063/1.5018130 [**Featured article**]

25. A. E. Boguslavskiy, O. Schalk, N. Gador, **WJG,** T. Mori, T. Schultz, M. S. Schuurman, T. J. Martínez, A. Stolow*, "Excited state non-adiabatic dynamics of the smallest polyene, *trans* 1,3-butadiene. I. Time-resolved photoelectron-photoion coincidence spectroscopy", *J. Chem. Phys.* **148**, 164302 (2018) https://doi.org/10.1063/1.5016452 [**Featured article**, Press release: https://publishing.aip.org/publishing/journal-highlights/missing-link-conducting-molecules-butadiene-solved]

24. C.-C. Zho, E. P. Farr, **WJG***, B. J. Schwartz*, "Temperature Dependence of the Hydrated Electron's Excited-State Relaxation I: Predictions of Cavity and Non-Cavity Mixed Quantum/Classical Simulation Models", *J. Chem. Phys.* **147**, 074503 (2017) http://dx.doi.org/10.1063/1.4985905

23. **WJG*** and B. J. Schwartz*, "Short-range Electron Correlation Stabilizes Non-cavity Solvation of the Hydrated Electron", *J. Chem. Theory Comput.* **12**, 5117 (2016) http://dx.doi.org/10.1021/acs.jctc.6b00472

22. J. R. Casey, B. J. Schwartz* and **WJG*,** "Free Energies of Cavity and Noncavity Hydrated Electrons Near the Instantaneous Air/water Interface", *J. Phys. Chem. Lett.* **7**, 3192 (2016) http://dx.doi.org/10.1021/acs.jpclett.6b01150

21. **WJG***, "Communication: Smoothing out excited-state dynamics: Analytical gradients for dynamically weighted complete active space self-consistent field", *J. Chem. Phys.* **141**, 171102 (2014) http://dx.doi.org/10.1063/1.4901328

20. **WJG**, J. R. Casey and B. J. Schwartz*, "Free Energies of Quantum Particles: The Coupled-Perturbed Quantum Umbrella Sampling Method", *J. Chem. Theory Comp.* **10**, 4661 (2014) http://dx.doi.org/10.1021/ct500661t

19. D. V. Makhov, **WJG**, T. J. Martínez* and D. V. Shalashilin*, "Ab Initio Multiple Cloning algorithm for quantum nonadiabatic molecular dynamics", *J. Chem. Phys.* **141**, 054110 (2014) http://dx.doi.org/10.1063/1.4891530

18. T. Kuhlman, **WJG**, T. Mori, K. Moller* and T. J. Martínez*, "Between Ethylenes and Polyenes – The Nonadiabatic Dynamics of cis-Dienes", *Faraday Disc.* **157**, 193 (2012) http://dx.doi.org/10.1039/C2FD20055D

17. T. Mori, **WJG**, M. S. Schuurman and T. J. Martínez*, "Role of Rydberg States in the Photochemical Dynamics of Ethylene", *J. Phys. Chem. A* **116**, 2808 (2012) http://dx.doi.org/10.1021/jp2097185

16. T. K. Allison, H. Tao, **WJG**, T. W. Wright, A. M. Stooke, C. Khurmi, J. van Tilborg, Y. Liu, R. W. Falcone, T. J. Martinez and A. Belkacem, "Ultrafast Internal Conversion in Ethylene. II. Mechanisms and Pathways for Quenching and Hydrogen Elimination", *J. Chem. Phys.* **136**, 124317 (2012) http://dx.doi.org/10.1063/1.3697760

15. **WJG**, R. E. Larsen and B. J. Schwartz*, "Simulating the Formation of Sodium:Electron Tight-Contact Pairs: Watching the Solvation of Atoms in Liquids One Molecule at a Time", *J. Phys. Chem. A* **115**, 5887 (2011) http://dx.doi.org/10.1021/jp1101434

14. R. E. Larsen, **WJG** and B. J. Schwartz*, "Response to Comments on 'Does the Hydrated Electron Occupy a Cavity?'" ***Science*** **331**, 1387-e (2011) http://dx.doi.org/10.1126/science.1197884

13. **WJG**, R. E. Larsen and B. J. Schwartz*, "Nature of Sodium Atoms/(Na^+,e^-) Contact Pairs in Liquid Tetrahydrofuran", *J. Phys. Chem. B*. **114**, 11535 (2010) http:// dx.doi.org/10.1021/jp103961j

12. R. E. Larsen, **WJG** and B. J. Schwartz*, "Does the Hydrated Electron Occupy a Cavity?", ***Science*** **329**, 65 (2010) http:// dx.doi.org/10.1126/science.1189588

11. A. E. Bragg, **WJG** and B. J. Schwartz*, "Watching the Solvation of Atoms in Liquids One Solvent Molecule at a Time", *Phys. Rev. Lett.* **104**, 233005 (2010) http://dx.doi.org/10.1103/PhysRevLett.104.233005

10. **WJG**, R. E. Larsen and B. J. Schwartz*, "First Principles Multi-electron Mixed Quantum/Classical Simulations in the Condensed Phase. II. The Charge-Transfer-to-Solvent States of Sodium Anions in Liquid Tetrahydrofuran", *J. Chem. Phys*. **132**, 144102 (2010) http://dx.doi.org/10.1063/1.3352564 [**Cover Article**]

9. **WJG**, R. E. Larsen and B. J. Schwartz*, "First Principles Multi-electron Mixed Quantum/Classical Simulations in the Condensed Phase. I. An Efficient Fourier-grid Method for Solving the Many-Electron Problem", *J. Chem. Phys*. **132**, 144101 (2010) http://dx.doi.org/10.1063/1.3352565 [**Top 20 downloads April 2010**]

8. **WJG**, R. E. Larsen and B. J. Schwartz*, "How does a solvent affect chemical bonds? Mixed quantum/classical simulations with a full CI treatment of the bonding electrons", *J. Phys. Chem. Lett*. **1**, 165-9 (2010) http://dx.doi.org/10.1021/jz9000938

7. R. E. Larsen, **WJG** and B. J. Schwartz*, "Comment on "An electron-water pseudopotential for condensed phase simulation" [J. Chem. Phys. 86, 3462 (1987)]", *J. Chem. Phys.* **131**, 037101 (2009) http://dx.doi.org/10.1063/1.3175801

6. **WJG**, R. E. Larsen and B. J. Schwartz*, "The roles of electronic exchange and correlation in charge-transfer-to-solvent dynamics: Many-electron nonadiabatic mixed quantum/classical simulations of photoexcited sodium anions in the condensed phase", *J. Chem. Phys.* **129**, 164505 (2008) http://dx.doi.org/10.1063/1.2996350

5. I. A. Shkrob*, **WJG**, R. E. Larsen and B. J. Schwartz*, "The structure of the hydrated electron. Part 2. A mixed quantum/classical molecular dynamics (MQC MD) – embedded cluster density functional theory: single-excitation configuration interaction (DFT:CIS) study", *J. Phys. Chem. A* **111**, 5232 (2007) http://dx.doi.org/10.1021/jp0682816

4. C. J. Smallwood, C. N. Mejia, **WJG**, R. E. Larsen and Benjamin J. Schwartz*, "A computationally efficient exact pseudopotential method. II. Application to the molecular pseudopotential of an excess electron interacting with tetrahydrofuran (THF)", *J. Chem. Phys.* **125**, 074103 (2006) http://dx.doi.org/10.1063/1.2218835

3. C. J. Smallwood, R. E. Larsen, **WJG** and B. J. Schwartz*, "A computationally efficient exact pseudopotential method. I. Analytic reformulation of the Phillips-Kleinman theory", *J. Chem. Phys.* **125**, 074102 (2006) http://dx.doi.org/10.1063/1.2218834

2. K. M. Carling, **WJG**, H. Gunaydin, T. A. Mitchell and E. A. Carter*, "Comparison of S, Pt, and Hf adsorption on NiAl(110)", *Surface Science* **600**, 2079 (2006) http://dx.doi.org/10.1016/j.susc.2006.02.047

1. **WJG** and P. A. Madden*, "Raman spectra of ionic liquids: A simulation study of $LaCl_3$ and its mixtures with alkali chlorides", *J. Chem. Phys.* **121**, 7293 (2004) http://dx.doi.org/10.1063/1.1792574

Contributed talks

2009/08/19 American Chemical Society National meeting, Washington, USA
2009/01/30 Western Spectroscopy Association, Asilomar, USA
2008/08/19 American Chemical Society National meeting, Philadelphia, USA
2008/07/23 American Conference on Theoretical Chemistry, Northwestern University, USA
2006/09/10 American Chemical Society National meeting, San Francisco, USA