

Curriculum Vitae  
**Dr. Jeffrey M. McMahon**

---

Department of Physics and Astronomy, Washington State University  
PO Box 642814, Pullman, WA 99164-2814 USA  
+1(815)200-2455 • [jeffrey.mcmahon@wsu.edu](mailto:jeffrey.mcmahon@wsu.edu)  
<https://labs.wsu.edu/mcmahon/>

**RESEARCH INTERESTS:**

The development and application of novel theoretical and computational quantum many-body methods. Specific areas of recent interest include: for methods development: the application of high-dimensional integration methods from applied mathematics as well as machine-learning methods from computer science to physics; for applications: the electronic structure of condensed matter and quantum fluids and solids.

**EDUCATION:**

<b>Ph.D.</b> , Northwestern University	(2010)
<b>B.S.</b> , Western Washington University	(2005)

**APPOINTMENTS:**

<b>Assistant Professor</b> , Department of Physics and Astronomy, Washington State University	(2015–Present)
<b>Postdoctoral Fellow</b> , Department of Chemistry, Northwestern University	(2014–2015)
<b>Postdoctoral Fellow</b> , Department of Physics, University of Illinois at Urbana–Champaign	(2010–2014)
<b>Research Assistant</b> , Department of Chemistry, Northwestern University	(2006–2010)
<b>Resident Research Associate</b> , Center for Nanoscale Materials, Argonne National Laboratory	(2006–2010)
<b>Research Assistant</b> , Department of Chemistry, Western Washington University	(2002–2005)

**AWARDS & HONORS:**

<b>Identification as an Expert in Nanotechnology</b> , U.S. Department of Labor	(2014)
<b>Gordon Research Conference, Invited Speaker</b> , University of New England	(2012)
<b>Springer Thesis Prize for Outstanding Ph.D. Research</b> , Springer & Northwestern University	(2011)
<b>Materials Research Science and Engineering Center Fellowship</b> , Northwestern University	(2009–2010)
<b>Graduate Student Award in Computational Chemistry</b> , American Chemical Society	(2009)
<b>Graduate Student Award to Attend the 59<sup>th</sup> Lindau Meeting of Nobel Laureates</b> , Lindau, Germany	(2009)
<b>Materials Research Science and Engineering Center Fellowship</b> , Northwestern University	(2008–2009)
<b>Outstanding Presentation Award</b> , The Federation of Analytical Chemistry and Spectroscopy Societies Meeting	(2004)
<b>Analytical Chemistry Student of the Year</b> , Western Washington University	(2002–2003)

**Honor Roll**, Western Washington University (2001–2003)

**TEACHING:**

<b>Quantum Theory I</b> (Physics 550), Washington State University	(2016)
<b>Physics for Scientists and Engineers II</b> (Physics 202), Washington State University	(2016)
<b>Physics of the Solid State</b> (Physics 563), Guest Lecturer, Washington State University	(2015)
<b>Graduate Seminar</b> (Physics 501), Guest Lecturer, Washington State University	(2015–Present)
<b>First-Year Seminar I</b> (Physics 188), Guest Lecturer, Washington State University	(2015–Present)
<b>Accelerated General Chemistry Labs</b> (Chemistry 171 and 172), Northwestern University	(2006)
<b>Polymer Chemistry Lab</b> (Chemistry 308), Western Washington University	(2005)
<b>Organic Chemistry Labs</b> (Chemistry 354 and 355), Western Washington University	(2003–2004)
<b>General Chemistry Labs</b> (Chemistry 121, 122, and 123), Western Washington University	(2002–2003)

**ADVISING:****Postdoctoral Fellows:**

Keeper L. Sharkey (2016–Present)

**Graduate Students:**

Praveer Tiwari	(2016–Present)
Craig M. Tenney	(2016–Present)
Jeevake Attapattu	(2015–Present)
Thomas L. Badman	(2015–Present)

**Undergraduate Students:**

Kenneth T. Haak	(2016–Present)
Zachary Croft	(2016–Present)
Andrew I. H. Cannon	(2016–Present)
Nikolas I. Steckley	(2015)
(Currently: Software Development Engineer at DiscoverOrg)	
Vera D. Prytkova	(2008)
(Currently: Ph.D. candidate at the University of California, Irvine)	

**COMMITTEES:**

**Department of Physics and Astronomy Colloquium**, Organizer, Washington State University (2016–Present)

**Center for Institutional Research Computing**, Member of the Advisory Committee and Chair of the Growth and Sustainability Subcommittee, Washington State University (2016–Present)

**Pacific Northwest Supercomputing Center** (proposed), Committee Member, Washington State University (2015–2016)

**Student-hosted Physical Chemistry Seminar**, Co-organizer, Northwestern University (2008)

**Department of Chemistry Colloquium**, Co-organizer,  
Northwestern University (2005–2006)

**American Chemical Society Chemistry Club**, Vice President,  
Western Washington University (2003–2004)

#### PROFESSIONAL MEMBERSHIPS:

**American Physical Society**, Member

**American Physical Society**, Division of Chemical Physics, Member

#### PROFESSIONAL SERVICES:

##### **Proposal Reviewer:**

*Government Grand Challenge programs*

##### **Manuscript Reviewer:**

*Science*

*Reviews of Modern Physics*

*Physical Review Letters*

*Physical Review B*

*Chemical Reviews*

*ACS Nano*

*Journal of Physical Chemistry C*

*Physical Chemistry Chemical Physics*

*Computer Physics Communications*

*Applied Physics Letters*

*Annalen der Physik*

*Optics Express*

*Journal of Chemical Physics*

*Journal of Nanoparticle Research*

*EPL (Europhysics Letters)*

*Solid State Sciences*

*Physica Status Solidi B*

*Solid State Communications*

*Phase Transitions*

*Progress In Electromagnetics Research*

##### **Conference Organization:**

**Session L35: General Contributed: Theory and Simulations of Materials in Extreme Conditions**,  
APS March Meeting, Chair, New Orleans, LA (2017)

**Technical session: Frontiers in Plasmonic Materials**,  
XXIV International Materials Research Congress meeting, Co-organizer, Cancún, Mexico (2015)

**PUBLICATIONS:****Manuscripts in Preparation:**

5. C. M. Tenney, Z. Croft, and J. M. McMahon, "Metallic hydrogen: A liquid superconductor?," *In Preparation* (2017)
4. C. M. Tenney, K. L. Sharkey, and J. M. McMahon, "On the possibility of metastable metallic hydrogen," *In Preparation* (2017)
3. J. M. McMahon, "On the matrix derivatives of matrix mechanics," *In Preparation* (2017)
2. J. Attapattu and J. M. McMahon, "Functionals and their derivatives from deep learning," *In preparation* (2017)
1. T. L. Badman and J. M. McMahon, "Ground-state phase diagram of  $^4\text{He}$  adsorption on flat graphene/graphite," *In Preparation* (2017)

**Manuscripts Submitted:**

2. J. M. McMahon, "Density functionals from deep learning," *Submitted* (2017); <https://arxiv.org/abs/1608.00316>
1. J. M. McMahon, R. C. Clay, III, M. A. Morales, C. Pierleoni, and D. M. Ceperley, "Melting line of atomic hydrogen from free-energy calculations," *Submitted* (2017)

**Peer-reviewed Publications:**

32. M. O. McAnally, J. M. McMahon, R. P. Van Duyne, and G. C. Schatz, "Coupled wave equations theory of surface-enhanced femtosecond stimulated Raman scattering," *The Journal of Chemical Physics* **145**, 094106 (2016); DOI: 10.1063/1.4961749
31. J. M. McMahon, G. C. Schatz, and S. K. Gray, "Correction: Plasmonics in the ultraviolet with the poor metals Al, Ga, In, Sn, Tl, Pb, and Bi," *Physical Chemistry Chemical Physics* **17**, 19670–19671 (2015); DOI: 10.1039/C5CP90112J
30. J. J. Foley, IV, J. M. McMahon, G. C. Schatz, H. Harutyunyan, G. P. Wiederrecht, and S. K. Gray, "Inhomogeneous Surface Plasmon Polaritons," *ACS Photonics* **1**, 739–745 (2014); DOI: 10.1021/ph500172f; arXiv: 1312.2029
29. M. A. Morales, J. R. Gergely, J. McMinis, J. M. McMahon, J. Kim, and D. M. Ceperley, "Quantum Monte Carlo benchmark of exchange-correlation functionals for bulk water," *Journal of Chemical Theory and Computation* **10**, 2355–2362 (2014); DOI: 10.1021/ct500129p
28. R. C. Clay, III, J. McMinis, J. M. McMahon, C. Pierleoni, D. M. Ceperley, and M. A. Morales, "Benchmarking exchange-correlation functionals for hydrogen at high pressures using quantum Monte Carlo," *Physical Review B* **89**, 184106 (2014); DOI: 10.1103/PhysRevB.89.184106
27. J. M. McMahon, G. C. Schatz, and S. K. Gray, "Plasmonics in the ultraviolet with the poor metals Al, Ga, In, Sn, Tl, Pb, and Bi," *Physical Chemistry Chemical Physics* **15**, 5415–5423 (2013); DOI: 10.1039/C3CP43856B
26. M. A. Morales, J. M. McMahon, C. Pierleoni, and D. M. Ceperley, "Towards a predictive first-principles description of solid molecular hydrogen with density functional theory," *Physical Review B* **87**, 184107 (2013); Editor's Suggestion; DOI: 10.1103/PhysRevB.87.184107
25. M. A. Morales, J. M. McMahon, C. Pierleoni, and D. M. Ceperley, "Nuclear Quantum Effects and Nonlocal Exchange-Correlation Functionals Applied to Liquid Hydrogen at High Pressure," *Physical Review Letters* **110**, 065702 (2013); DOI: 10.1103/PhysRevLett.110.065702
24. J. M. McMahon, M. A. Morales, C. Pierleoni, and D. M. Ceperley, "The properties of hydrogen and helium under extreme conditions," *Reviews of Modern Physics* **84**, 1607–1653 (2012); Cover Article; DOI: 10.1103/RevModPhys.84.1607

23. J. M. McMahon, S. Li, L. K. Ausman, and G. C. Schatz, "Modeling the Effect of Small Gaps in Surface-Enhanced Raman Spectroscopy," *Journal of Physical Chemistry C* **116**, 1627–1637 (2012); DOI: 10.1021/jp207661y
22. J. M. McMahon and D. M. Ceperley, "Erratum: High-temperature superconductivity in atomic metallic hydrogen," *Physical Review B* **85**, 219902(E) (2012); DOI: 10.1103/PhysRevB.85.219902
21. J. M. McMahon, "Ground-state structures of ice at high pressures from *ab initio* random structure searching," *Physical Review B* **84**, 220104(R) (2011); DOI: 10.1103/PhysRevB.84.220104; arXiv:1106.1941v1
20. J. M. McMahon and D. M. Ceperley, "High-temperature superconductivity in atomic metallic hydrogen," *Physical Review B* **84**, 144515 (2011); DOI: 10.1103/PhysRevB.84.144515; arXiv:1106.5526v1
19. J. M. McMahon and D. M. Ceperley, "Ground-State Structures of Atomic Metallic Hydrogen," *Physical Review Letters* **106**, 165302 (2011); DOI: 10.1103/PhysRevLett.106.165302; arXiv:1011.5028v1
18. J. M. McMahon, S. K. Gray, and G. C. Schatz, "Fundamental behavior of electric field enhancements in the gaps between closely spaced nanostructures," *Physical Review B* **83**, 115428 (2011); DOI: 10.1103/PhysRevB.83.115428; arXiv:1008.2490v2
17. J. M. McMahon, S. K. Gray, and G. C. Schatz, "Optical Properties of Nanowire Dimers with a Spatially Nonlocal Dielectric Function," *Nano Letters* **10**, 3473–3481 (2010); DOI: 10.1021/nl101606j
16. H. Chen, J. M. McMahon, M. A. Ratner, and G. C. Schatz, "Classical Electrodynamics Coupled to Quantum Mechanics for Calculation of Molecular Optical Properties: A RT-TDDFT/FDTD Approach," *Journal of Physical Chemistry C* **114**, 14384–14392 (2010); DOI: 10.1021/jp1043392
15. S. Peng, J. M. McMahon, G. C. Schatz, S. K. Gray, and Y. Sun, "Reversing the size-dependence of surface plasmon resonances," *Proceedings of the National Academy of Sciences of the United States of America* **107**, 14530–14534 (2010); DOI: 10.1073/pnas.1007524107
14. J. M. McMahon, S. K. Gray, and G. C. Schatz, "Calculating nonlocal optical properties of structures with arbitrary shape," *Physical Review B* **82**, 035423 (2010); DOI: 10.1103/PhysRevB.82.035423; arXiv:0912.4746v2
13. K. L. Wustholz, A.-I. Henry, J. M. McMahon, R. G. Freeman, N. Valley, M. E. Piotti, M. J. Natan, G. C. Schatz, and R. P. Van Duyne, "Structure–Activity Relationships in Gold Nanoparticle Dimers and Trimers for Surface-Enhanced Raman Spectroscopy," *Journal of the American Chemical Society* **132**, 10903–10910 (2010); DOI: 10.1021/ja104174m
12. E. Ringe\*, J. M. McMahon\*, K. Sohn, C. Cobley, Y. Xia, J. Huang, G. C. Schatz, L. D. Marks, and R. P. Van Duyne, "Unraveling the Effects of Size, Composition, and Substrate on the Localized Surface Plasmon Resonance Frequencies of Gold and Silver Nanocubes: A Systematic Single-Particle Approach," *Journal of Physical Chemistry C* **114**, 12511–12516 (2010); DOI: 10.1021/jp104366r
11. J. M. McMahon, S. K. Gray, and G. C. Schatz, "Nonlocal Dielectric Effects in Core–Shell Nanowires," *Journal of Physical Chemistry C* **114**, 15903–15908 (2010); DOI: 10.1021/jp910899b
10. T. W. Odom, H. Gao, J. M. McMahon, J. Henzie, and G. C. Schatz, "Plasmonic superlattices: Hierarchical subwavelength hole arrays," *Chemical Physics Letters* **483**, 187–192 (2009); DOI: 10.1016/j.cplett.2009.10.084
9. J. M. McMahon, S. K. Gray, and G. C. Schatz, "Nonlocal optical response of metal nanostructures with arbitrary shape," *Physical Review Letters* **103**, 097403 (2009); DOI: 10.1103/PhysRevLett.103.097403. *Virtual Journal of Nanoscale Science & Technology* **20**, 10 (2009)
8. J. M. McMahon, A.-I. Henry, K. L. Wustholz, M. J. Natan, R. G. Freeman, R. P. Van Duyne, and G. C. Schatz, "Gold nanoparticle dimer plasmonics: finite element method calculations of the electromagnetic enhancement to surface-enhanced Raman spectroscopy," *Analytical and Bioanalytical Chemistry* **394**, 1819–1825 (2009); DOI: 10.1007/s00216-009-2738-4
7. H. Gao, J. M. McMahon, M. H. Lee, J. Henzie, S. K. Gray, G. C. Schatz, and T. W. Odom, "Rayleigh anomaly-surface plasmon polariton resonances in palladium and gold subwavelength hole arrays," *Optics Express* **17**, 2334–2340 (2009); DOI: 10.1364/OE.17.002334

6. Y. Babayan, J. M. McMahon, S. Li, S. K. Gray, G. C. Schatz, and T. W. Odom, "Confining Standing Waves in Optical Corrals," *ACS Nano* **3**, 615–620 (2009); DOI: 10.1021/nn8008596
5. J. M. McMahon, S. K. Gray, and G. C. Schatz, "A discrete action principle for electrodynamics and the construction of explicit symplectic integrators for linear, non-dispersive media," *Journal of Computational Physics* **228**, 3421–3432 (2009); DOI: 10.1016/j.jcp.2009.01.019
4. J. M. McMahon, Y. Wang, L. J. Sherry, R. P. Van Duyne, L. D. Marks, S. K. Gray, and G. C. Schatz, "Correlating the Structure, Optical Spectra, and Electrodynamics of Single Silver Nanocubes," *Journal of Physical Chemistry C* **113**, 2731–2735 (2009); DOI: 10.1021/jp8098736
3. J. Zhao, A. O. Pinchuk, J. M. McMahon, S. Li, L. K. Ausman, A. L. Atkinson, and G. C. Schatz, "Methods for Describing the Electromagnetic Properties of Silver and Gold Nanoparticles," *Accounts of Chemical Research* **41**, 1710–1720 (2008); DOI: 10.1021/ar800028j
2. J. M. McMahon, J. Henzie, T. W. Odom, G. C. Schatz, and S. K. Gray, "Tailoring the sensing capabilities of nanohole arrays in gold films with Rayleigh anomaly-surface plasmon polaritons," *Optics Express* **15**, 18119–18129 (2007); DOI: 10.1364/OE.15.018119. *Virtual Journal of Nanoscale Science & Technology* **17**, 10 (2008)
1. J. M. McMahon and S. R. Emory, "Phase Transfer of Large Gold Nanoparticles to Organic Solvents with Increased Stability," *Langmuir* **23**, 1414–1418 (2007); DOI: 10.1021/la0617560

**Book:**

1. J. M. McMahon, *Topics in Theoretical and Computational Nanoscience: From Controlling Light at the Nanoscale to Calculating Quantum Effects with Classical Electrodynamics* (Springer: New York, NY 2011); DOI: 10.1007/978-1-4419-8249-0; ISBN: 978-1-4419-8248-3

**Book Chapters:**

5. J. M. McMahon, S. K. Gray, and G. C. Schatz, "FDTD Computation of the Nonlocal Optical Properties of Arbitrarily Shaped Nanostructures", In: A. Taflove (ed), *Advances in FDTD Computational Electrodynamics: Photonics and Nanotechnology* (Artech House: USA 2013); ISBN: 978-1-60807-170-8
4. H. Chen, J. M. McMahon, M. A. Ratner, and G. C. Schatz, "Classical Electrodynamics Coupled to Quantum Mechanics for Calculation of Molecular Optical Properties: An RT-TDDFT/FDTD Approach", In: A. Taflove (ed), *Advances in FDTD Computational Electrodynamics: Photonics and Nanotechnology* (Artech House: USA 2013); ISBN: 978-1-60807-170-8
3. N. Harris, L. K. Ausman, J. M. McMahon, D. J. Masiello, and G. C. Schatz, "Computational Electrodynamics Methods," In: E. Bichoutskaia (ed), *Computational Nanoscience* (The Royal Society of Chemistry: Cambridge, UK 2011); ISBN: 978-1-84973-133-1
2. J. M. McMahon, S. K. Gray, and G. C. Schatz, "Surface Nanophotonics Theory," In: G. Wiederrecht (ed), *Handbook of Nanoscale Optics and Electronics* (Elsevier: Amsterdam 2010); Cover Image; ISBN: 978-0-12-375178-2
1. A. L. Atkinson, J. M. McMahon, and G. C. Schatz, "FDTD Studies of Metallic Nanoparticle Systems," In: *Self Organization of Molecular Systems, From Molecules and Clusters to Nanotubes and Proteins, NATO Science for Peace and Security Series A: Chemistry and Biology* (Springer: Netherlands 2009); DOI: 10.1007/978-90-481-2590-6

**Conference Proceedings:**

2. J. M. McMahon, S. K. Gray, and G. C. Schatz, "Dephasing of Electromagnetic Fields in Scattering from an Isolated Slit in a Gold Film," *Proceedings of SPIE* **7033**, 703311/1–6 (2008); DOI: 10.1117/12.790647
1. G. C. Schatz, J. M. McMahon, and S. K. Gray, "Tailoring the parameters of nanohole arrays in gold films for sensing applications," *Proceedings of SPIE* **6641**, 664103/1–8 (2007); DOI: 10.1117/12.731368

**INVITED PRESENTATIONS:**

11. Z. Croft, C. M. Tenney, and J. M. McMahon, "Metallic Hydrogen: A Liquid Superconductor?," (poster) Academic Showcase, Washington State University (March 2017)
10. A. I. H. Cannon, K. T. Haak, and J. M. McMahon, "Inside Neptune-like Planets from First Principles," (poster) Academic Showcase, Washington State University (March 2017)
9. J. M. McMahon, "On the Molecular Dissociation of Dense Hydrogen and the Finite-temperature Stability of the Atomic Phase," Department of Chemistry, Washington State University (October 2016)
8. J. M. McMahon, "On the Molecular Dissociation of Dense Hydrogen and the Finite-temperature Stability of the Atomic Phase," Department of Physics, University of Idaho (April 2016)
7. J. M. McMahon, "From Shining Light on the Nanoscale to Taking Materials to the Extreme," Department of Chemistry, University of Cincinnati (November 2014)
6. J. M. McMahon, M. A. Morales, C. Pierleoni, and D. M. Ceperley, "On the Molecular Dissociation of Dense Hydrogen and the Finite-Temperature Stability of the Atomic Phase," Department of Physics, Rutgers University (April 2013)
5. J. M. McMahon and D. M. Ceperley, "Predicting the Properties of Ordinary Matter Under Extreme Conditions," 16<sup>th</sup> International Workshop on Computational Physics and Materials, Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy (January 2013)
4. J. M. McMahon, M. A. Morales, C. Pierleoni, and D. M. Ceperley, "On the Molecular Dissociation of Dense Hydrogen and the Finite-Temperature Stability of the Atomic Phase," Gordon Research Conference, University of New England (June 2012)
3. J. M. McMahon, M. A. Morales, C. Pierleoni, and D. M. Ceperley, "On the Molecular Dissociation of Dense Hydrogen and the Finite-Temperature Stability of the Atomic Phase," ES12, Wake Forest University (June 2012)
2. J. M. McMahon and G. C. Schatz, "Determining the Nonlocal Optical Properties of Metallic Nanostructures via High-Performance Computing," HPCNano09 at SC09, Portland, OR (November 2009)
1. J. M. McMahon and G. C. Schatz, "Computational Nanophotonics: Applications of Classical Electrodynamics to Nanoscience," The Elsevier Seminar, The Ohio State University, Department of Chemistry, Columbus, OH (May 2009)

**CONTRIBUTED PRESENTATIONS (SINCE 8/16/2015):**

5. J. M. McMahon, "On the Possibility of Metastable Metallic Hydrogen," APS March Meeting, New Orleans, LA (March 2017)
4. A. I. H. Cannon, K. T. Haak, and J. M. McMahon, "Inside Neptune-like Planets from First Principles," (poster) Gordon Research Conference, Research at High Pressure, Holderness School (July 2016)
3. J. M. McMahon, "Density Functionals from Deep Learning," (poster) Academic Showcase, Washington State University (March 2016)
2. J. M. McMahon, "Density Functionals from Deep Learning," APS March Meeting, Baltimore, MD (March 2016)
1. J. M. McMahon, "Nonlocal Dielectric Effects in Core–Shell Nanowires," XXIV International Materials Research Congress meeting, Cancún, Mexico (August 2015)