

ADAM PHILLIP WILLARD

Curriculum Vitae

Massachusetts Institute of Technology
Department of Chemistry
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Education:

Ph.D.	University of California, Berkeley	Chemistry	2009
B.S.	University of Puget Sound	Chemistry and Mathematics	2003

Research and Professional Experience:

Associate Professor, Department of Chemistry, Massachusetts Institute of Technology	2018-Present
Assistant Professor, Department of Chemistry, Massachusetts Institute of Technology	2013-2018
Postdoctoral Fellow, University of Texas at Austin (Peter Rossky)	2010-2013
Postdoctoral Fellow, Lawrence Berkeley National Laboratory (David Chandler)	2009-2010
Graduate Student, University of California, Berkeley (David Chandler)	2004-2009

Honors and Awards:

OpenEye Outstanding Junior Faculty Award	2018
Scialog Fellow: Advanced Energy Storage	2017
Cottrell Scholar Award	2016
NSF CAREER Award	2015

Undergraduate Students Supervised:

Duplessi, Kyle; Summer	2019	
Hedley, Jonathan; Summer	2019	
Chen, Songela; UROP	2017-2019	currently: D.E. Shaw Research
Gunderman, Lane, UROP	2014-2015	currently: Ph.D. Student, Waterloo Physics
Latham, Andrew, Summer	2016	currently: Ph.D. Student, MIT Chemistry

PH.D. Students Supervised:

Maria Alejandra Castellanos Morales, *in progress*
Ardavan Farahvash, *in progress*
Aditya Limaye, *in progress*
Yizhi Shen, *in progress*
Kyaw Myint, *in progress*
Dodin, Amr, *in progress*
Dwelle, Kaitlyn, *in progress*
Avila, Thomas, *in progress*
Alt, Eric, 2019 “Structural modeling of dynamic polymer networks”
Lee, Chee Kong, 2018 “Simulating exciton dynamics in organic semiconductors”

Lee, Elizabeth, 2018 “Nonequilibrium energy transport in molecular semiconductors”
Shin, Sucheol, 2018 “Orientational fluctuations of liquid water at hydrophobic and hydrophilic interfaces”, current position: postdoc, UT Austin

Postdoctoral Researchers Supervised:

Ding, Wendu 2018-present
Hiscock, Hamish 2018-present
Neisen, Micheil 2018-present
Teichen, Paul 2015-2018 Senior research engineer, Etiometry
Shi, Liang, 2014-2016 Assistant Professor, University of California, Merced
Kattirtzi, John, 2014-2015 Postdoc, Jun Cheng Group, Aberdeen UK

Teaching Experience:

5.60, Thermodynamics, Statistical Mechanics, and Kinetics, Spring 2017-2018, Fall 2019
5.70, Statistical Thermodynamics, Fall 2013-2016, 2018

Service:

Internal:

Chair, Physical Chemistry Seminar Series 2013-2014
Co-Chair, Physical Chemistry Seminar Series 2014-present
Graduate Admissions Committee 2013-present
Junior Faculty Search Committee 2013-2017
Undergraduate Advisor 2013-2017, 2019-present

External:

Early Career Editorial Advisor Board, Journal of Chemical Physics 2019-present
Co-organizer, Greater Boston Area Statistical Mechanics Meeting 2013-present
Co-organizer, ACS symposium “Supramolecular Aggregates” March 2016

Ad hoc Review: *Journal of the American Chemical Society*, *Journal of Physical Chemistry*, *Physical Review Letters*, *Journal of Chemical Physics*, *Journal of Physical Chemistry Letters*, *Journal of Chemical Theory and Computation*, *Physical Review A*, *Nature Chemistry*, *Proceedings of the National Academy of Science*, *Nature Communication*, *Langmuir*, *ACS Central Science*, *Chem*, *Physical Chemistry Chemical Physics*, *ACS Petroleum Research Fund*, *U.S. Department of Energy*, *U.S. National Science Foundation*

Consulting:

2016 Akita Innovation

Publications:

1. A. Dodin and **A. P. Willard**, “State-space distribution and dynamical flow for closed and open quantum systems”, *J. Chem. Phys.*, 151, 064106, (2019).
2. E. M. Y. Lee and **A. P. Willard**, “Solving the trivial crossing problem while preserving the nodal symmetry of the wavefunction”, *J. Chem. Theo. Comp.*, 15(8), 4332-4343, (2019).
3. R. H. Gilmore, Y. Liu, W. Wu, N. S. Dahod, E. M.Y. Lee, M. C. Weidman, H. Li, J. Jean, V. Bulovic, **A. P. Willard**, J. C. Grossman, W. A. Tisdale, "Epitaxial Dimers and Auger-Assisted Detrapping in PbS Quantum Dot Solids." *Matter*, 1, 250-265, (2019).

4. C.K. Lee, L. Shi, and **A. P. Willard**. "Modeling the Influence of Correlated Molecular Disorder on the Dynamics of Excitons in Organic Molecular Semiconductors." *J. Phys. Chem. C*, 123(1), 306-314, (2019).
5. E. M. Y. Lee, W. A. Tisdale, and **A. P. Willard**. "Perspective: Nonequilibrium dynamics of localized and delocalized excitons in colloidal quantum dot solids." *J. Vac. Sci. Tec. A*, 36(6), 068501, (2018).
6. L. Shi and **A. P. Willard**, "Modeling the effects of molecular disorder on the properties of Frenkel excitons in organic molecular semiconductors", *J. Chem. Phys.* 149, 094110, (2018).
7. R. H. Gilmore, S. W. Winslow, E. M. Y. Lee, M. Nickol Ashner, K. G. Yager, **A. P. Willard**, and W. A. Tisdale, "Inverse Temperature Dependence of Charge Carrier Hopping in Quantum Dot Solids", *ACS Nano*, 12(8), 7741-7749, (2018).
8. S. Shin and **A. P. Willard**, "Water's Interfacial Hydrogen Bonding Structure Reveals the Effective Strength of Surface-Water Interactions", *J. Phys. Chem. B*, 122(26), 6781-6789, (2018).
9. Y. Gu, E. A. Alt, H. Wang, X. Li, **A. P. Willard**, and J. A. Johnson, "Photoswitching Polymer Network Topology", *Nature*, 560, 65-69, (2018).
10. S. Shin and **A. P. Willard**, "Three-body Hydrogen Bond Defects Contribute Significantly to the Dielectric Properties of the Liquid Water-Vapor Interface", *J. Phys. Chem. Lett.*, 9(7), 1649-1654, (2018).
11. M. S. Azzaro, A. Dodin, D. Y. Zhang, **A. P. Willard**, and S. T. Roberts. "Exciton-Delocalizing Ligands Can Speed Energy Migration in Nanocrystal Solids.", *Nano letters.*, 18(5), 3259–3270, (2018).
12. S. Shin and **A. P. Willard**, "Characterizing Hydration Properties Based on the Orientational Structure of Interfacial Water Molecules", *J. Chem. Theo. Comp.* 14(2), 461-465, (2018).
13. M. R. Golder, Y. Jiang, P. E. Teichen, H. V.-T. Nguyen, W. Wang, N. Milos, S. A. Freedman, **A. P. Willard**, J. A. Johnson, "Stereochemical Sequence Dictates Unimolecular Diblock Copolymer Assembly", *J. Am. Chem. Soc.* 140(5), 1596-1599, (2018).
14. F. S. Freyria, J. Cordero, J. Caram, S. Doria, A. Dodin, **A. P. Willard**, and M. Bawendi "Near-Infrared Quantum Dot Emission Enhanced by Stabilized Self-Assembled J-Aggregate Antennas", *Nano Lett.*, 17(12), 7665-7674, (2017).
15. L. Shi, C. K. Lee, and **A. P. Willard**, "The Enhancement of Interfacial Exciton Dissociation by Energetic Disorder is a Nonequilibrium Effect", *ACS Cent. Sci.*, 3(12), 1262-1270, (2017).
16. A. J. Goodman, **A. P. Willard**, and W. A. Tisdale, "Exciton trapping is responsible for the long apparent lifetime in acid-treated MoS₂", *Phys. Rev. B.*, 96, 121404, (2017).
17. J. A. Kattirtzi, D. T. Limmer, and **A. P. Willard**, "Microscopic dynamics of charge separation at the aqueous electrochemical interface", *Proc. Nat. Acad. Sci.*, 114, 13374-13379, (2017).
18. E. M. Y. Lee, A. J. Mork, **A. P. Willard**, and W. A. Tisdale, "Including surface ligand effects in continuum elastic models of nanocrystal vibrations", *J. Chem. Phys.*, 147, 044711, (2017).
19. R.H. Gilmore, E.M.Y. Lee, M.C. Weidman, **A. P. Willard**, and W.A. Tisdale, "Charge Carrier Hopping Dynamics in Homogeneously Broadened PbS Quantum Dot Solids", *Nano Lett.*, 17, 893-901, (2017).
20. A.J. Mork, E.M.Y. Lee, N.S. Dahod, **A. P. Willard**, and W.A. Tisdale, "Modulation of Low-Frequency Acoustic Vibrations in Semiconductor Nanocrystals through Choice of Surface Ligand", *J. Phys. Chem. Lett.*, 7, 4213–4216, (2016).
21. A.V. Zhukhovitskiy, J. Zhao, M. Zhong, E.G. Keeler, E.A. Alt, P.E. Teichen, R.G. Griffin, M.J. Hore, **A. P. Willard**, J.A. Johnson, "Polymer Structure Dependent Hierarchy in PolyMOC Gels", *Macromolecules*, 49, 6896–6902, (2016).
22. C. K. Lee, L. Shi, and **A. P. Willard**, "A Model of Charge Transfer Excitons: Diffusion, Spin Dynamics, and Magnetic Field Effects", *J. Phys. Chem. Lett.*, 7, 2246-2251, (2016).
23. A.V. Zhukhovitskiy, M. Zhong, E.G. Keeler, V.K. Michaelis, J.E.P. Sun, M.J. A. Hore, D.J. Pochan, R.G. Griffin, **A. P. Willard**, J.A. Johnson, "High branch functionality and loop-rich polymer metal-organic cage gels." *Nature Chem.*, 8, 33-41, (2016).
24. P. B. Deotare, W. Chang, E. Hontz, D. N. Congreve, L. Shi, P. D. Reusswig, B. Modtland, M. E. Bahlke, C. K. Lee, **A. P. Willard**, V. Bulović, T. Van Voorhis, and M. A. Baldo, "Nanoscale transport of charge transfer states in organic donor-acceptor blends." *Nature Mat.*, 14, 1130-1134, (2015).

25. B. Reeja-Jayan, N. Chen, J. Lau, J.A. Kattirtzi, P. Moni, A. Liu, I.G. Miller, R. Kayser, **A. P. Willard**, B. Dunn, K. K. Gleason, "A group of cyclic siloxane and silazane polymer films as nanoscale electrolytes for microbattery architectures." *Macromolecules*, 48(15), 5222-5229, (2015).
26. E.M.Y. Lee, W.A. Tisdale, and **A. P. Willard**, "Can disorder enhance incoherent exciton diffusion?" *J. Phys. Chem. B*, 119,9501-9509, (2015).
27. **A. P. Willard**, "Illuminating the Interactions between Small Solutes in Liquid Water." *J. Phys. Chem. Lett.*, 6(9), 1616-1617, (2015).
28. D.T. Limmer and **A. P. Willard**, "Nanoscale heterogeneity at the aqueous electrolyte-electrode interface," *J. Chem. Phys. Lett.*, 620, 144-150, (2015).
29. G.M. Akselrod, F. Prins, L.V. Poulikakos, E.M.Y. Lee, M.C. Weidman, A.J. Mork, **A. P. Willard**, V. Bulović, and W.A. Tisdale, "Subdiffusive Exciton Transport in Quantum Dot Solids," *Nano Lett.*, 14(6), 3556-3562, (2014).
30. P. Varilly, **A. P. Willard**, J. B. Kirkegaard, T. P. J. Knowles, and D. Chandler "Intra-chain organisation of hydrophobic residues controls inter-chain aggregation rates of amphiphilic polymers", *J. Chem. Phys.*, 146, 135102, (2017).
31. D.T. Limmer, **A. P. Willard**, P.A. Madden, and D. Chandler, "Water Exchange at a Hydrated Platinum Electrode Is Rare and Collective", *J. Phys. Chem. C*, 119, 24016, (2015).
32. Z. Hu, **A. P. Willard**, R.J. Ono, C.W. Bielawski, P.J. Rossky and D.A. Vanden Bout, "The nature of interchain excited states in polythiophene: excitonic vs. charge-transfer character." *Nature Comm.*, 6, 8246, (2015).
33. **A. P. Willard** and D. Chandler, "The molecular structure of the interface between water and a hydrophobic substrate is liquid-vapor like," *J. Chem. Phys.* 141(18), 18C519, (2014).
34. **A. P. Willard**, D.T. Limmer, P.A. Madden, and D. Chandler, "Characterizing heterogeneous dynamics at hydrated electrode surfaces," *J. Chem. Phys.*, 138, 184702, (2013).
35. D.T. Limmer, **A. P. Willard**, P.A. Madden, and D. Chandler, "Hydration of metal surfaces can be dynamically heterogeneous and hydrophobic," *Proc. Nat. Acad. Sci.*, 110, 4200-4205, (2013).
36. A.E. Jailaubekov, **A. P. Willard**, J.R. Tritsch, W.-L. Chan, N. Sai, R. Gearba, L.G. Kaake, K.J. Williams, K. Leung, P.J. Rossky, and X.-Y. Zhu, "Hot Charge Transfer Excitons Set the Time Limit for Charge Separation at Donor/Acceptor Interfaces in Organic Photovoltaics," *Nature Mat.*, 12, 66-73, (2012).
37. R. Vacha, O. Marsalek, **A. P. Willard**, D.J. Bonthuis, R.R. Netz, and P. Jungwirth, "Charge Transfer between Water Molecules As the Possible Origin of the Observed Charging at the Surface of Pure Water," *J. Phys. Chem. Lett.*, 3, 107-111, (2012).
38. **A. P. Willard**, and D. Chandler, "Instantaneous Liquid Interfaces," *J. Phys. Chem. B*, 114, 1954-1958, (2010).
39. **A. P. Willard**, S.K. Reed, P.A. Madden, and D. Chandler, "Water at an Electrochemical Interface--a Simulation Study," *Faraday Discussion*, 141, 423-441, (2009).
40. **A. P. Willard**, and D. Chandler, "Coarse Grained Modeling of the Interface Between Water and Heterogeneous Surfaces," *Faraday Discussion*, 141, 209-220, (2009).
41. **A. P. Willard**, and D. Chandler, "The Role of Solvent Fluctuations in Hydrophobic Assembly," *J. Phys. Chem. B*, 112, 6187-6192, (2008).

Submitted Publications:

1. A. M. Limaye and **A. P. Willard**, "Modeling interfacial electron transfer in the double layer: interplay between electrode coupling and electrostatic driving", *ACS Central Science*, submitted, (2019).
2. K. Dwelle and **A. P. Willard**, "Constant potential, electrochemically active boundary conditions for electrochemical simulation", *J. Phys. Chem. C*, under revision, (2019).
3. A. Dodin, B. Aull, R. R. Kunz, and **A. P. Willard**, "Theoretical bounds on electron energy filtering in disordered nano materials", *Nano. Lett.*, under revision, (2019).