

CURRICULUM VITAE

Yulia Pushkar

Department of Physics and Astronomy, Purdue University
525 Northwestern Avenue West Lafayette, IN 47907
Phone: 765-4963279 Email: ypushkar@purdue.edu

Academic preparation

Postdoc: 2004-2008, University of California, Berkeley & Lawrence Berkeley National Lab.

Postdoc: 2003-2004, Institut für Experimentalphysik, Freie Universität Berlin, Germany.

Ph.D. 2003 (summa cum laude), Biophysics, Freie Universität Berlin, Germany.

M.S. 1999 (with honor), Physical Chemistry, Moscow State University, Russia.

Appointments

Professor of Physics Purdue University	2020 - present
Associate Professor of Physics Purdue University	2014 - 2020
Visiting Professor, Swiss Federal Institute of Technology (ETH, Zurich)	05-11, 2015
Assistant Professor of Physics Purdue University	2008 - 2014

Awards:

Society of the Sigma Xi: full member	2021
Showalter Faculty Scholar	2019
Purdue College of Science Team Award (for work on T32 Molecular Biophysics Training Grant)	2019
Outstanding Advisor Award, Purdue University	2017
The Purdue College of Science Research Award	2016
Kavli Fellow (promising young scientist under the age of 40)	2015
Outstanding Advisor Award, Purdue University	2015
National Science Foundation CAREER Award	2014
Seed for Success Award, Purdue University (for attracting over one million dollars in research funding)	2010
Young Investigator Award, Gordon Research Conference on Photosynthesis	2006
Postdoctoral Richard Malkin Award for research in the field of photosynthesis	2005
The German Academic Exchange Service (DAAD) grant for graduate study	2000
Halder-Topsoe Graduate Student Research Grant	1999
Chevron Corporation Award for Research in Ecologically Friendly Catalysis	1998
Open Society Institute and Soros Foundation Undergraduate Research Grants	1994-1999

Experience

- 26+ years of experimental experience in EPR spectroscopy as applied in catalysis; molecular biophysics; protein studies; studies of the electron transfer process in proteins, protein-cofactor interactions. Experience in spin labels, isotope labels and paramagnetic probe molecules techniques.
- 19+ years of experimental experience in application of synchrotron X-ray absorption, emission and diffraction methods for analysis of molecular structures; crystal structures; structure and function of active sites in metalloproteins; electronic structures of organic/inorganic compounds. Optical pump-probe and time resolved studies using lasers

and X-rays.

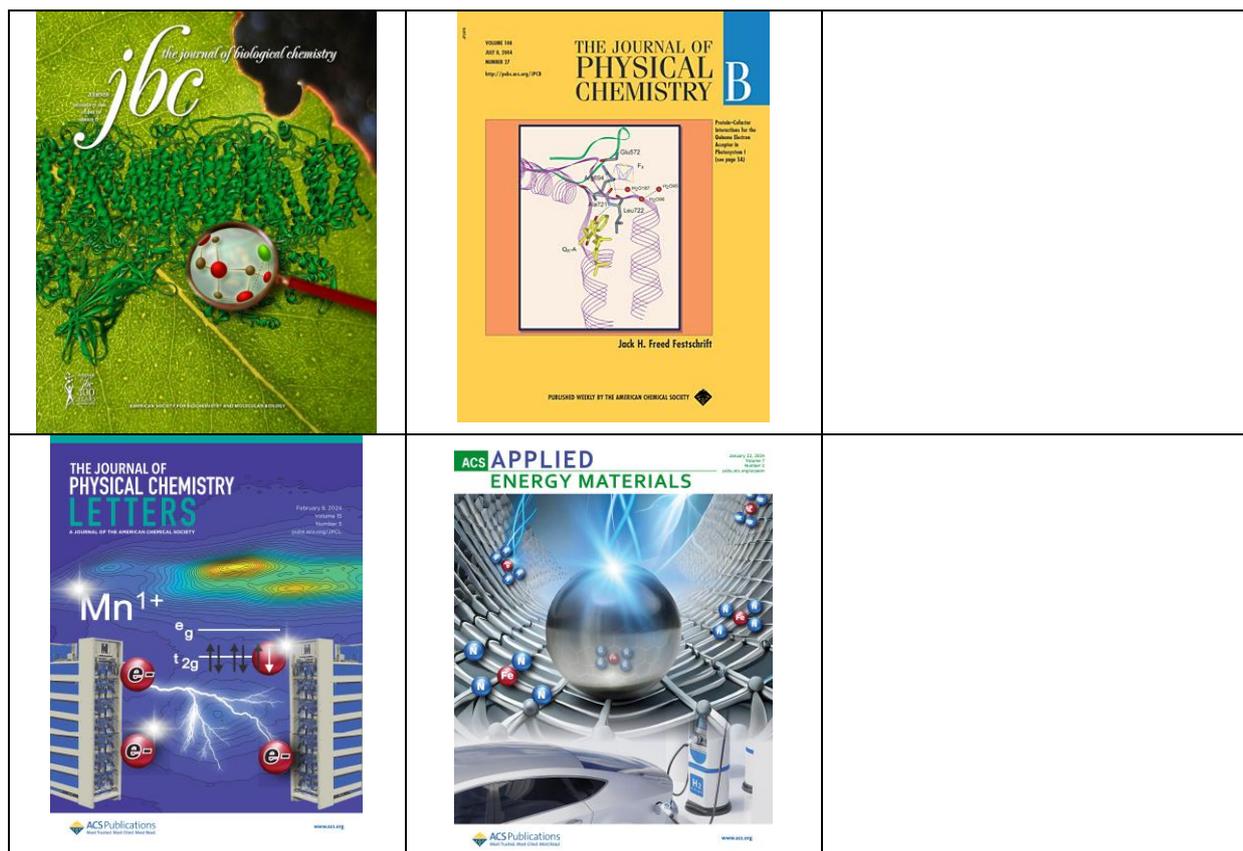
- 15+ years of experience in computational DFT modeling and analysis of molecular structures, mechanisms, and spectroscopic responses.
- 15+ years of experience in brain imaging and studies of molecular mechanisms of neurodegeneration.

Synergistic activities

- Member: American Chemical Society, Biophysical Society
- Co-organizer of Midwest Photosynthesis Meeting
- Manuscript reviewer for Journal of the American Chemical Society, Nature Chemistry, Nature Energy, Nature Catalysis, Angewandte Chemie, Biochemistry, Materials Today, Polyhedron, The Journal of Physical Chemistry, PlosOne, Inorganic Chemistry, ACS catalysis, Brain Structure, Chem. Soc. Rev., ChemSUSChem, ChemComm, Metallomics, Journal of Biological Inorganic Chemistry, PCCP, Cell Reports Methods, Journal of Synchrotron Radiation; European Journal of Inorganic Chemistry, Molecules, Exploration of Neuroprotective Therapy, Pharmaceutics, Computational and Theoretical Chemistry, Neurotoxicity Research.
- Reviewer of grants for: DOE, NSF (panel on protein interactions, structure and design; panel on chemistry of life processes, catalysis), NIH, Austrian Science Fund; Petroleum Research Foundation, Israel Science Foundation, Sir Henry Wellcome postdoctoral fellowships; Paul Scherrer Institute (Switzerland) Equipment grants; Netherlands Organization for Scientific Research
- Member of Spectroscopy panel, Advanced Photon Source, ANL (2015-2022)
- Reviewer of beamtime proposals for SSRL and CHESS (2009-present)
- Faculty Member, Purdue Quantum Science and Engineering Institute

List of publications





1. “Challenges of observing O-O bond formation in the Mn₄Ca cluster of Photosystem II”
Scott Jensen, Brendan T. Sullivan, Daniel A. Hartzler, Irina Kosheleva¹, Robert W. Henning¹, Allison Page, and Yulia Pushkar, *Chem*, 2025, accepted
2. "Spectroscopic Signature of Metal -hydroxo and peroxy Species in K-edge X-ray Absorption Spectra"
Olga Maximova, Roman Ezhov, Scott Jensen, Cheng-Jun Sun, Yulia Pushkar, *The Journal of Physical Chemistry Letters*, 2024, 15 (44), 11077-11086.
3. "Metal-Dependent Electrocatalytic Oxygen Reduction in Surface-Conjugated Macrocyclic Electrodes"
Moumita Ghosh, Roman Ezhov, Sarah Braley, Yaroslav Losovyj, Gabriel Bury, Yulia Pushkar, Jeremy Smith, *ACS Applied Energy Materials*, 2024, 7(15), 6717-6726.
4. „Insights from Ca²⁺→Sr²⁺ Substitution on the Mechanism of O-O bond formation in Photosystem II”
Gabriel Bury, Yulia Pushkar, *Photosynthesis Research*, 2024, 1-21.
5. “Rational design of improved Ru containing Fe-based Metal-Organic Framework (MOF) photoanode for artificial photosynthesis”
Jully Patel, Gabriel Bury, Yulia Pushkar, *Small*, 2024, 2310106 (1-13p).
6. “Evaluation of Ce-MOFs as photoanode materials for water oxidation reaction, effect of doping with [Ru(bpy)(dcbpy)(H₂O)₂]²⁺ catalyst”
Naduvile Purayil Dileep, Jully Patel, Yulia Pushkar, *Inorganic Chemistry*, 2024, 63 (18), 8050-8058.
7. “Spectroscopic Characterization of Mn¹⁺ Low Oxidation State in Prussian Blue-Based Battery Anodes”
Olga Maximova, Winter Allen, Grace Yee, Charlotte Israel, Denis Leshchev, Eli Stavitski, Yujia Ding, Katherine Davis, Colin Wessells, Daniel Friebe, and Yulia Pushkar, *The Journal of Physical Chemistry Letters*, 2024, 15, 5, 1521–1528.

This paper was featured on the journal cover.

8. “Pentanuclear iron complex for water oxidation: spectroscopic analysis of reactive intermediates in solution and catalyst immobilization into the MOF-based photoanode”

Roman Ezhov, Gabriel Bury, Olga Maximova, Elliot Daniel Grant, Mio Kondo, Shigeyuki Masaoka, Yulia Pushkar, *Journal of Catalysis*, 2023, v. 429, pp 115230.

9. "Spectroscopic Characterization of Highly Active Fe-N-C Oxygen Reduction Catalyst and Discovery of Strong Interaction with Nafion Ionomer"
Roman Ezhov, Olga Maximova, Xiang Lyu, Denis Leshchev, Eli Stavitski, Alexey Serov, Yulia Pushkar, *ACS Applied Energy Materials*, 2024, 7, 2, 604–613.

This paper was featured on the journal cover.

10. "Revisit the E2 Domain of Amyloid Precursor Protein: Ferroxidase, Superoxide and Peroxynitrite Scavenging Activities"
Andrew Poore, Eli Zuercher, Gabriel Bury, Caslyn Whitesell, Cuong Nguyen, Yulia Pushkar, Shiliang Tian, *Inorganic Chemistry*, 2023, 62, 27, 10780–10791.
11. "High-resolution imaging of Hg/Se aggregates in the brain of small Indian mongoose, a wild terrestrial species: insights into intracellular Hg detoxification"
Pavani Devabathini, Darrell L Fischer, Si Chen, Ajith Pattammattel, Gabriel Bury, Olga Antipova, Xiaojing Huang, Yong S Chu, Sawako Horai, Yulia Pushkar, *Environmental Chemistry Letters*, 2023, 1-6.
12. "Photoexcitation of Fe₃O nodes in MOF drives water oxidation at pH= 1 when Ru catalyst is present"
Roman Ezhov, Alireza K Ravari, Mark Palenik, Alexander Loomis, Debora M Meira, Sergey Savikhin, Yulia Pushkar, *ChemSusChem*, 2023, e202202124.
13. "X-ray Emission Spectroscopy of Single Protein Crystals Yields Insights into Heme Enzyme Intermediates"
Sahand Emamian, Kendra A Ireland, Vatsal Purohit, Kirklín L McWhorter, Olga Maximova, Winter Allen, Scott Jensen, Diego M Casa, Yulia Pushkar, Katherine M Davis, *Journal of Physical Chemistry Letters*, 2023, 14, 1, 41–48.
14. "A Manganese Compound I Model with a High Reactivity in the Oxidation of Organic Substrates and Water"
Lina Zhang, Mi Sook Seo, Yunhee Choi, Roman Ezhov, Olga Maximova, Deesha D Malik, Maggie Ng, Yong-Min Lee, Ritimukta Sarangi, Yulia N Pushkar, Kyung-Bin Cho, Wonwoo Nam, *Journal of the American Chemical Society*, 2023, 145, 15, 8319–8325.
15. "A Spectroscopically Observed Iron Nitrosyl Intermediate in the Reduction of Nitrate by a Surface-Conjugated Electrocatalyst"
Moumita Ghosh, Sarah Braley, Roman Ezhov, Harrison Worster, Juan Valdez-Moreira, Yaroslav Losovyj, Elena Jakubikova, Yulia Pushkar, Jeremy Smith, *Journal of the American Chemical Society*, 2022, 144, 39, 17824–17831.
16. "Computational Analysis of Structure–Activity Relationships in Highly Active Homogeneous Ruthenium-Based Water Oxidation Catalysts"
Gabriel Bury, Yulia Pushkar, *Catalysts*, 2022, 12, 863.
17. "Systematic influence of electronic modification of ligand on the catalytic rate of water oxidation by a single-site Ru-based catalyst"
Jully Patel, Gabriel Bury, Alireza K Ravari, Roman Ezhov, Yulia Pushkar, *ChemSusChem*, 2022 15, e2021016.
18. "Do multi-nuclear 3d metal catalysts achieve O-O bond formation via radical coupling or via water nucleophilic attack? WNA leads the way in [Co₄O₄]⁴⁺"
Roman Ezhov, Alireza Karbakhsh Ravari, Gabriel Bury, Paul F. Smith, Yulia Pushkar, *Chem Catalysis*, 1, 1-16, 2021.
19. "A Highly Reactive Chromium(V)-Oxo TAML Cation Radical Complex in Electron Transfer and Oxygen Atom Transfer Reactions"
Young Hyun Hong, Yuri Jang,; Roman Ezhov, Mi Sook Seo, Yong-Min Lee, Bhawana Pandey, Seungwoo Hong, Yulia Pushkar, Shunichi Fukuzumi, Nam, Wonwoo, *ACS Catalysis*, 2021, 11, 2889-2901.
20. "A Mononuclear Nonheme Iron(III)-Peroxo Complex with an Unprecedented High O-O Stretch and Electrophilic Reactivity"

- Wenjuan Zhu, Semin Jang, Jin Xiong, Roman Ezhov, Xiao-Xi Li, Taeyeon Kim, Mi Sook Seo, Yong-Min Lee, Yulia Pushkar, Ritimukta Sarangi, Yisong Guo, Nam, Wonwoo, *Journal of the American Chemical Society*, 2021, 143, 38, 15556–15561.
21. “Facile Light-Induced Transformation of $[\text{Ru}^{\text{II}}(\text{bpy})_2(\text{bpyNO})]^{2+}$ to $[\text{Ru}^{\text{II}}(\text{bpy})_3]^{2+}$ ” Alireza K. Ravari, Yuliana Pineda-Galvan, Alexander Huynh, Roman Ezhov, Yulia Pushkar, *Inorganic Chemistry*, 2020, 59 (19), 13880-13887.
 22. "Atomically-dispersed Iridium on Indium Tin Oxide Efficiently Catalyzes Water Oxidation" Dmitry Lebedev, Roman Ezhov, Javier Heras-Domingo, Aleix Comas-Vives, Nicolas Kaeffer, Marc Willinger, Xavier Solans-Monfort, Xing Huang, Yulia Pushkar, Christophe Copéret, *ACS Central Science*, 2020, 6, 1189-1198.
 23. “Characterization of the $\text{Fe}^{\text{V}}=\text{O}$ complex in the pathway of water oxidation” Roman Ezhov, Alireza Karbakhsh Ravari, Yulia Pushkar, *Angewandte Chemie*, 2020, 132, 13604-13607.
 24. „Water Oxidation Catalyst $\text{cis-}[\text{Ru}(\text{bpy})(5,5'\text{-dcbpy})(\text{H}_2\text{O})_2]^{2+}$ and Its Stabilization in Metal-organic Framework” Roman Ezhov, Alireza Ravari Karbakhsh, Allison Page, Yulia Pushkar, *ACS Catalysis*, 2020, 10, 5299-5308.
 25. „Unraveling the mechanism of catalytic water oxidation via *de novo* synthesis of reactive intermediate“ Alireza Karbakhsh Ravari, Guibo Zhu, Roman Ezhov, Yuliana Pineda-Galvan, Allison Baily Page, Whitney Weinschenk, Lifen Yan, Yulia Pushkar, *Journal of the American Chemical Society*, 2020, 142(2), 884-893.
 26. „An evolutionarily conserved iron-sulfur cluster underlies redox sensory function of the Chloroplast Sensor Kinase“ Iskander M. Ibrahim, Huan Wu, Roman Ezhov, Gilbert E. Kayanja, Stanislav D. Zakharov, Yanyan Du, Weiguo Andy Tao, Yulia Pushkar, William A. Cramer, and Sujith Puthiyaveetil, *Communications Biology*, 2020, 3(1), 1-11.
 27. “A High-Valent Manganese(IV)-Oxo-Ce(IV) Complex and Its Enhanced Oxidizing Reactivity“ Deepika G. Karmalkar, Muniyandi Sankaralingam, Mi Sook Seo, Roman Ezhov, Yong-Min Lee, Yulia N. Pushkar, Won-Suk Kim, Shunichi Fukuzumi, and Wonwoo Nam, *Angewandte Chemie*, 2019, 131, 1-7.
 28. „Early Binding of Substrate Oxygen is Responsible for Spectroscopically Distinct S_2 -State in Photosystem II“ Yulia Pushkar, Alireza Karbakhsh Ravari, Scott Jensen, Mark C Palenik, *Journal of Physical Chemistry Letters*, 2019, 10,17, 5284-5291.
 29. „Detection of the site protected 7-coordinate $\text{Ru}^{\text{V}}=\text{O}$ species and its chemical reactivity to enable catalytic water oxidation” Yuliana Pineda-Galvan, Alireza K. Ravari, Sergei Shmakov, Liubov Lifshits, Nattawat Kaveevivitchai, Randolph Thummel, Yulia Pushkar, *Journal of Catalysis*, 2019, 375, 1-7.
 30. „Redox Reactivity of a Mononuclear Manganese-Oxo Complex Binding Calcium Ion and Other Redox-Inactive Metal Ions“ Muniyandi Sankaralingam, Yong-Min Lee, Yuliana Pineda-Galvan, Deepika G Karmalkar, Mi Sook Seo, So Hyun Jeon, Yulia Pushkar, Shunichi Fukuzumi, Wonwoo Nam, *Journal of the American Chemical Society*, 2019, 141 (3), pp 1324–1336
 31. “DIY XES - Development of an Inexpensive, Versatile, and Easy to Fabricate XES Analyzer and Sample Delivery System” Scott C. Jensen, Brendan T. Sullivan, Daniel A. Hartzler, and Yulia Pushkar, *X-ray Spectrometry*, 2019, 1-9.
 32. „X-ray Emission Spectroscopy at X-ray Free Electron Lasers: Limits to Observation of the Classical Spectroscopic Response for Electronic Structure Analysis“ S. Jensen, B. T. Sullivan, D. A. Hartzler, J. M. Aguilar, S. Awel, S. Bajt, S. Basu, R. Bean, H. Chapman, C. Conrad, M. Frank, R. Fromme, J. M. Martin-Garcia, T. D. Grant, M. Heymann, M. S. Hunter, G. Ketawala, R. A. Kirian, J. Knoska, C. Kupitz, X. Li, M. Liang, S. Lisova, V. Mariani, V. L. Mazalova, M. Messerschmidt, M. Moran, G. Nelson, D. Oberthuer, A. Schaffer, R. G. Sierra, N. Vaughn, U. Weierstall,

- M. O. Wiedorn, P. L. Xavier, J.-H. Yang, O. Yefanov, N. Zatsépin, A. L. Aquila, P. Fromme, S. Boutet, G. T. Seidler, Y. Pushkar, *The Journal of Physical Chemistry Letters*, 2019, 10 (3), pp 441–446.
33. „Mechanism for O-O bond formation via radical coupling of metal and ligand based radicals – a new pathway“
Yulia Pushkar, Yuliana Pineda-Galvan, Alireza K. Ravari, Tatiana Otroshchenko, Daniel A. Hartzler, *Journal of the American Chemical Society*, 2018, 140, (42), 13538-13541.
 34. “Rapid evolution of the Photosystem II electronic structure during water splitting“
Katherine M. Davis, Brendan T. Sullivan, Mark Palenik, Lifan Yan, Vatsal Purohit, Gregory Robison, Irina Kosheleva, Robert W. Henning, Gerald T. Seidler, Yulia Pushkar, *Physical Review X*, 2018, 8, 041014.
 35. “Model of the Oxygen Evolving Complex which is highly predisposed to O–O bond formation “
Yulia Pushkar, Katherine M. Davis, Mark Palenik, *The Journal of Physical Chemistry Letters*, 2018, 9, 3524-3531.
 36. “The key Ru^V=O intermediate of site-isolated mononuclear water oxidation catalyst detected by *in situ* X-ray absorption spectroscopy”
Dmitry Lebedev, Yuliana Pineda-Galvan, Yuki Tokimaru, Alexey Fedorov, Nicolas Kaeffer, Christophe Copéret and Yulia Pushkar, *Journal of the American Chemical Society*, 2018, 140, 451-458.
 37. “Insights into MOF Reactivity: Chemical Water Oxidation Catalysis by a [Ru(tpy)(dcbpy)OH₂]²⁺ Modified Metal-Organic Framework”
Shaoyang Lin, Alireza K. Ravari, Pavel M. Usov, Meng Cai, Jie Zhu, Spencer R. Ahrenholtz, Yulia Pushkar, Amanda J. Morris, *ChemSusChem*, 2018, 11, 464. DOI: 10.1002/cssc.201701644.
 38. “X-ray Emission Spectroscopy of Biomimetic Mn Coordination Complexes”
Scott C. Jensen, Katherine M. Davis, Brendan Sullivan, Daniel A. Hartzler, Gerald T. Seidler, Diego M. Casa, Elina Kasman, Hannah E. Colmer, Allyssa A. Massie, Timothy A. Jackson, and Yulia Pushkar, *The Journal of Physical Chemistry Letters*, 2017, 8, 2584–2589.
 39. “Electrochemical Water Oxidation by a Catalyst-Modified Metal Organic Framework Thin Film”
Shaoyang Lin, Yuliana P. Galvan, William A. Maza, Charity C. Epley, Jie Zhu, Matthew C. Kessinger, Yulia Pushkar, Amanda J. Morris, *ChemSusChem*, 2017, 10, 3, 514-522.
- This paper was featured on the journal cover.
40. „On the nature of the Cu-rich aggregates in brain astrocytes“
Brendan Sullivan, Gregory Robison, Jenna Osborn, Martin Kay, Peter Thompson, Katherine Davis, Taisiya Zakharova, Olga Antipova, Yulia Pushkar, *Redox Biology*, 2017, v. 11, 231-239
 41. Mechanistic Analysis of Water Oxidation Catalyst *cis*-[Ru(bpy)₂(H₂O)₂]²⁺: Effect of Dimerization.
Darren Erdman, Yuliana Pineda-Galvan and Yulia Pushkar, *Catalysts*, 2017, v. 7 (2) article number 39.
 42. “X-ray emission spectroscopy of Mn coordination complexes towards interpreting the electronic structure of the Oxygen Evolving Complex of Photosystem II”
Katherine M. Davis, Mark Palenik, Lifan Yan, Paul F. Smith, Gerald T. Seidler, G. Charles Dismukes, Yulia Pushkar, *Journal of Physical Chemistry C*, 2016, 120(6), 3326-3333.
 43. „*In vivo* Mn exposure does not affect adult neurogenesis in rats“
Brendan Sullivan, Gregory Robison, Martin Kay, Yulia Pushkar, *Toxicological Sciences*, 2016, 152(2): 257-61.
 44. „Copper Accumulation in Rodent Brain Astrocytes: A Species Difference”
Brendan Sullivan, Gregory Robison, John K. Young, Kebreten F. Manaye, Yulia Pushkar, *Journal of Trace Elements in Medicine and Biology*, 2017; 39: 6-13.
 45. „Uncovering the role of oxygen atom transfer in Ru-based catalytic water oxidation“
Dooshaye Moonshiram, Yuliana Pineda-Galvan, Darren Erdman, Mark Palenik, Ruifa Zong, Randolph Thummel, Yulia Pushkar *Journal of the American Chemical Society*, 2016, 138 (48), pp 15605–15616.

46. „Rapid Evolution of the Photosystem II Electronic Structure during Water Splitting“
Katherine M. Davis, Brendan T. Sullivan, Mark Palenik, Lifan Yan, Vatsal Purohit, Gregory Robison, Irina Kosheleva, Robert W. Henning, Gerald T. Seidler, Yulia Pushkar, [arXiv:1506.08862](https://arxiv.org/abs/1506.08862)
47. “Unexpected Ligand Lability in Condition of Water Oxidation Catalysis”
Lifan Yan, Ruifa Zong, Yulia Pushkar, *Journal of Catalysis*, 2015, V. 330, p. 255-260.
48. “Structure of the Oxygen Evolving Complex of Photosystem II at Room Temperature”
Katherine M. Davis, Yulia Pushkar, *Journal of Physical Chemistry B*, 2015, 119(8), p. 3492-3498.
49. “Identification of dopaminergic neurons of the substantia nigra compacta as a target of manganese accumulation”
Gregory A. Robison; Brendan Sullivan; Jason R Cannon; Yulia Pushkar, *Metallomics*, 2015, 7(5), p. 748-755, 10.1039/C5MT00023H.
- This paper was featured on the journal cover.
50. „Spectroscopic analysis of catalytic water oxidation by $\text{Ru}^{\text{II}}(\text{bpy})(\text{tpy})\text{H}_2\text{O}]^{2+}$ suggests that $\text{Ru}^{\text{V}}=\text{O}$ is not a rate-limiting intermediate“
Yulia Pushkar, Dooshaye Moonshiram, Vatsal Purohit, Lifan Yan, Igor Alperovich, *Journal of the American Chemical Society*, 2014, 136 (34), pp 11938–11945.
51. “Serial Time-resolved crystallography of Photosystem II using a femtosecond X-ray laser”
C. Kupitz, S. Basu, I. Grotjohann, R. Fromme, N. A. Zatsepin, K. N. Rendek, M. Hunter, R. L. Shoeman, T. A. White, D. Wang, D. James, J.-H. Yang, D. E Cobb, B. Reeder, R. G. Sierra, H. Liu, A. Barty, A. L. Aquila, D. Deponte, R. A. Kirian, S. Bari, J. J. Bergkamp, K. R. Beyerlein, M. J. Bogan, C. Caleman, T.-C. Chao, C. E. Conrad, K. M. Davis, H. Fleckenstein, L. Galli, S. P. Hau-Riege, S. Kassemeyer, H. Laksmono, M. Liang, L. Lomb, S. Marchesini, A. M. Martin, M. Messerschmidt, D. Milathianaki, K. Nass, A. Ros, S. Roy-Chowdhury, K. Schmidt, M. Seibert, J. Steinbrener, F. Stellato, L. Yan, C. Yoon, T. A. Moore, A. L. Moore, Y. Pushkar, G. J. Williams, S. Boutet, R. B. Doak, U. Weierstall, M. Frank, H. N. Chapman, J. C.H. Spence and P. Fromme, *Nature*, 2014, 513, pp 261-265.
52. „Triplet excited state energies and phosphorescence spectra of (bacterio)chlorophylls.“
Daniel A. Hartzler, Dariusz M. Niedzwiedzki, Donald A. Bryant, Robert E. Blankenship, Yulia Pushkar, Sergei Savikhin, *Journal of Physical Chemistry B*, 2014, 118 (26), pp 7221–7232.
53. “Electronic structure assessment: Combined Density Functional Theory Calculations and Ru $L_{2,3}$ -edge X-ray Absorption Near-edge Spectroscopy of Water Oxidation Catalyst”
Igor Alperovich, Dooshaye Moonshiram, Javier Concepcion, and Yulia Pushkar, *Journal of Physical Chemistry C*, 2013, 117 (37), pp 18994–19001.
54. „X-ray Fluorescence Imaging of the Hippocampal Formation after Manganese Exposure”
Gregory Robison, Taisiya Zakharova, Sherleen X. Fu, Wendy Jiang, Rachael Fulper, Raul Barrea, Wei Zheng and Yulia Pushkar, *Metallomics*, 2013, 5 (11), pp 1554-1565.
55. “Kinetic modeling of the x-ray induced damage to a metalloprotein”
Katherine M. Davis, Irina Kosheleva, Robert W. Henning, Gerald T. Seidler, Yulia Pushkar, *Journal of Physical Chemistry B*, 2013, 117 (31), pp 9161–9169.
56. “Aging results in copper accumulations in GFAP-positive cells in the subventricular zone”
Yulia Pushkar, Gregory Robison, Brendan Sullivan, Wei Zheng, Sherleen X. Fu, Meghan Kohne, Wendy Jiang, Sven Rohr, Barry Lai, Matthew A. Marcus, Taisiya Zakharova, *Aging Cell*, 2013, 12(5), pp 823–832. DOI: 10.1111/acer.12112.
57. „Electronic Structure Changes of Mn in the Oxygen-Evolving Complex of Photosystem II during the Catalytic Cycle“
Pieter Glatzel, Henning Schroeder, Yulia Pushkar, Thaddeus Boron, Shreya Mukherjee, George Christou, Vincent L. Pecoraro, Johannes Messinger, Vittal K. Yachandra, Uwe Bergmann, and Junko Yano, *Inorganic Chemistry*, 2013, 52 (10), pp 5642–5644.

58. „Mechanism of Catalytic Water Oxidation by Ruthenium Blue dimer catalyst: comparative study in D₂O versus H₂O“
Dooshaye Moonshiram, Vatsal Purohit, Javier Concepcion, Thomas Meyer, Yulia Pushkar, *Materials*, 2013, 6 (2), pp 392-409.
59. „Experimental Demonstration of Radicaloid Character in a Ru^V=O Intermediate in Catalytic Water Oxidation“
Dooshaye Moonshiram, Igor Alperovich, Javier Concepcion, Thomas Meyer, Yulia Pushkar, *Proceedings of the National Academy of Science*, 2013 110 (10) 3765-3770.
60. “A Mononuclear Nonheme Manganese(IV)-Oxo Complex Binding Redox-Inactive Metal Ions.”
Junying Chen, Yong-Min Lee, Katherine M. Davis, Xiujuan Wu, Mi Sook Seo, Kyung-Bin Cho, Heejung Yoon, Young Jun Park, Shunichi Fukuzumi, Yulia N. Pushkar, and Wonwoo Nam, *Journal of the American Chemical Society*, 2013, 135 (17), pp 6388–6391.

This paper was featured on the journal cover.

61. “X-ray Fluorescence Imaging: A New Tool for Studying Manganese Neurotoxicity”
Gregory Robison, Taisiya Zakharova, Sherleen X. Fu, Rachel Fulper, Wendy Jiang, Matthew A. Marcus, Raul Barrea, Wei Zheng, Yulia Pushkar, *PlosOne*, 2012, Vol. 7 (11), Article Number: e48899.
62. “Ru L_{2,3} XANES theoretical simulation with DFT: a test of the core-hole treatment”
Igor Alperovich, Dooshaye Moonshiram, Alexander Soldatov, Yulia Pushkar, *Solid State Communications*, 2012, V.152, 1880-1884.
63. “Increased β-Amyloid Deposition in Tg-SWDI Transgenic Mouse Brain Following In Vivo Lead Exposure“, Huiying Gu, Gregory Robison, Raul Barrea, Xing Wei, Martin R. Farlow, Yulia Pushkar, Yansheng Du, Wei Zhen, *Toxicology Letters*, 2012, Vol. 213, 211-219.
64. “Fast detection Allowing Analysis of the Electronic Structure of Metalloprotein by X-ray Emission Spectroscopy at Room Temperature”
Katherine M. Davis, Brian A. Mattern, Joseph I. Pacold, Taisiya Zakharova, Dale Brewere, Irina Kosheleva, Robert W. Henning, Timothy J. Graber, Steve M. Heald, Gerald T. Seidler, Yulia Pushkar, *Journal of Physical Chemistry Letters*, 2012, 3, 1858–1864.
65. “Theoretical modelling of L_{2,3}-edges XANES using DFT”
Igor Alperovich, Alexander Soldatov, Dooshaye Moonshiram, Yulia Pushkar, *Journal of Experimental and Theoretical Physics Letters*, 2012, v. 95, issue 10.
66. “Structure and Electronic Configurations of the Intermediates of Water Oxidation in Blue Ruthenium Dimer Catalysis“
Dooshaye Moonshiram, Jonah Jurss, Javier Concepcion, Taisiya Zakharova, Igor Alperovich, Thomas Meyer, Yulia Pushkar, *Journal of American Chemical Society*, 2012, 134, 4625-4636.
67. “A Highly Reactive Mononuclear Nonheme Manganese(IV)-Oxo Complex That Can Activate the Strong C-H Bonds of Alkanes”
Xiujuan Wu, Mi Sook Seo, Katherine Davis, Yong-Min Lee, Junying Chen, Kyung-Bin Cho, Yulia Pushkar, Wonwoo Nam, *Journal of American Chemical Society*, 2011, 133 (50), pp 20088–20091.
68. “Understanding the Electronic Structure of 4d Metal Complexes: From Molecular Spinors to L-edge Spectra of a di-Ru Catalyst”
Igor Alperovich, Grigory Smolentsev, Dooshaye Moonshiram, Jonah W. Jurss, Javier J. Concepcion, Thomas Meyer, Alexander Soldatov, Yulia Pushkar, *Journal of American Chemical Society*, 2011, 133 (39), p 15786–15794.
69. “Direct Detection of Oxygen Ligation to the Mn₄Ca Cluster of Photosystem II by X-ray Emission Spectroscopy“
Yulia Pushkar, Xi Long, Pieter Glatzel, Gary W. Brudvig, G. Charles Dismukes, Terrence J. Collins, Vittal K. Yachandra, Junko Yano, Uwe Bergmann, *Angewandte Chemie International Edition*, 2010, v. 49, 4, p 800-803.

- 70., „Activation of a water molecule using a mononuclear Mn complex: from Mn-aquo, to Mn-hydroxo, to Mn-oxyl via charge compensation“
Benedikt Lassalle-Kaiser, Christelle Hureau, Dimitrios A. Pantazis, Yulia Pushkar, Regis Guillot, Vittal K. Yachandra, Junko Yano, Frank Neese, Elodie Anxolabehere-Mallart, **Energy & Environmental Science**, 2010, v. 3, 7, 924-938
71. “X-ray Emission Spectroscopy To Study Ligand Valence Orbitals in Mn Coordination Complexes”
Grigoriy Smolentsev, Alexander V. Soldatov, Johannes Messinger, Kathrin Merz, Thomas Weyhermuller, Uwe Bergmann, Yulia Pushkar, Junko Yano, Vittal K. Yachandra, Pieter Glatzel, *Journal of American Chemical Society*, 2009, 131, 13161-13167.
72. “Incorporation of 2,3-Disubstituted-1,4-naphthoquinones into the A₁ Binding Site of Photosystem I Studied by EPR and ENDOR Spectroscopy“
Art van der Est, Yulia Puskar, Irina Karyagina, Branden Fonovic, Travis Dudding, Jens Niklas, Wolfgang Lubitz, John H. Golbeck, *Applied Magnetic Resonance*, 2010, 37, 65-83.
73. “Single-Molecule Magnetism Properties of the First Strontium-Manganese Cluster [SrMn₁₄O₁₁(OMe)₃(O₂CPh)₁₈(MeCN)₂]”
Abhodaya Mishra, Yulia Pushkar, Junko Yano, Vittal K. Yachandra, Wolfgang Wernsdorfer, Khalil A. Abboud, George Christou *Inorganic Chemistry* 2008, 47, 1940-1948.
74. “Visible Light-Induced Electron Transfer from Di- μ -oxo-Bridged Dinuclear Mn Complexes to Cr Centers in Silica Nanopores”
Walter Weare, Yulia Pushkar, Vittal Yachandra, Heinz Frei, *Journal of American Chemical Society* 2008, 130(34); 11355-11363.
75. “Structural changes in the Mn₄Ca cluster and the mechanism of photosynthetic water splitting”
Yulia Pushkar, Junko Yano, Kenneth Sauer, Alain Boussac, Vittal Yachandra *Proceedings of the National Academy of Science* 2008, vol. 105, N. 6, 1879-1884.
76. “High-resolution structure of the photosynthetic Mn₄Ca catalyst from X-ray spectroscopy”
Junko Yano, Jan Kern, Yulia Pushkar, Kenneth Sauer, Pieter Glatzel, Uwe Bergmann, Johannes Messinger, Athina Zouni, Vittal K. Yachandra *Philosophical Transactions of the Royal Society B* 2008 vol. 363, N. 1494, 1139-1147.
77. “Focusing the view on Nature’s water splitting catalyst”
Samir Zein, Leonid V. Kulik, Junko Yano, Jan Kern, Yulia Pushkar, Athina Zouni, Vittal K. Yachandra, Wolfgang Lubitz, Frank Neese, Johannes Messinger *Philosophical Transactions of the Royal Society B* 2008 vol. 363, N. 1494, 1167-1177.
78. “Polarized X-ray Absorption Spectroscopy of Single-Crystal Mn(V) Complexes Relevant to the Oxygen Evolving Complex of Photosystem II”
Junko Yano, John Robblee, Yulia Pushkar, Matthew A. Marcus, Jesper Bendix, Josè M. Workman, Terrence J. Collins, Edward I. Solomon, Serena DeBeer George, Vittal Yachandra *Journal of the American Chemical Society* 2007, 129(43), 12989-13000.
79. “Contributions of the Protein Environment to the Midpoint Potentials of the A₁ Phylloquinones and the F_X Iron-Sulfur Cluster in Photosystem I”
Irina Karyagina, Yulia Pushkar, Dietmar Stehlik, Art van der Est, Hiroshi Ishikita, Ernst-Walter Knapp, Bharat Jagannathan, Rufat Agalarov, and John H. Golbeck *Biochemistry* 2007, 46(38), 10804-10816.
80. “Structure and orientation of the Mn₄Ca cluster in plant Photosystem II membranes studied by polarized range-extended X-ray absorption spectroscopy”
Yulia Pushkar, Junko Yano, Pieter Glatzel, Johannes Messinger, Azul Lewis, Kenneth Sauer, Uwe Bergmann, Vittal K. Yachandra *Journal of Biological Chemistry* 2007, V. 282, N. 10, 7198-7208.

This paper was selected as a paper of the week by Journal of Biological Chemistry and featured on the journal cover

81. "Hetero nuclear Mn-Ca/Sr Complexes, and Ca/Sr EXAFS Spectral Comparisons with the Oxygen-Evolving Complex of Photosystem II"
Abhudaya Mishra, Junko Yano, Yulia Pushkar, Vittal K. Yachandra, Khalil A. Abboud, George Christou *Chemical Communications* 2007, V. 15, 1538-1540.
82. "Where Water is Oxidized to Oxygen: Structure of the Photosynthetic Mn₄Ca Cluster"
Junko Yano, Jan Kern, Kenneth Sauer, Matthew J. Latimer, Yulia Pushkar, Jacek Biesiadka, Bernhard Loll, Wolfram Saenger, Johannes Messinger, Athina Zouni, Vittal K. Yachandra *Science* 2006, V.314; 821-825
83. "High-Resolution Mn EXAFS of the Oxygen-Evolving Complex in Photosystem II: Structural Implications for the Mn₄Ca Cluster"
Junko Yano, Yulia Pushkar, Pieter Glatzel, Azul Lewis, Kenneth Sauer, Johannes Messinger, Uwe Bergmann, Vittal Yachandra *Journal of the American Chemical Society (Communication)* 2005, V. 127, N. 43, 14974-14975.
84. "X-ray Damage to the Mn₄Ca Complex in Single-Crystals of Photosystem II: A Case Study for Metallo-Protein Crystallography"
Junko Yano, Jan Kern, Klaus-Dieter Irrgang, Matthew J. Latimer, Uwe Bergmann, Pieter Glatzel, Yulia Pushkar, Jacek Biesiadka, Bernhard Loll, Kenneth Sauer, Johannes Messinger, Athina Zouni, Vittal K. Yachandra *Proceedings of the National Academy of Science* 2005, V. 102, N 34, 12047-12052.
85. "Recruitment of a Foreign Quinone into the A₁ site of Photosystem I. Consecutive Forward Electron Transfer from A₀ to A₁ to F_X with Anthraquinone in the A₁ Site as studied by transient EPR"
Yulia Pushkar, Irina Karyagina, Dietmar Stehlik, Sarah Brown, Art van der Est *Journal of Biological Chemistry* 2005, V. 280, N13, 12382-12390.
86. "Recruitment of a Foreign Quinone into the A₁ site of Photosystem I. Characterization of a *menB rubA* double deletion mutant in *Synechococcus SP.* PCC 7002 devoid of F_X, F_A and F_B and containing Plastoquinone or exchanged 9,10-Anthroquinone"
Yumiko Sakuragi, Boris Zybailov, Gaozhong Shen, Donald A. Bryant, John H. Golbeck, Bruce A. Diner, Irina Karyagina, Yulia Pushkar, and Dietmar Stehlik *Journal of Biological Chemistry* 2005, V. 280, N13, 12371-12381.
87. "Transient and pulsed EPR study of ¹⁷O substituted methyl-naphthoquinone as radical anion in the A₁ binding site of Photosystem I and in frozen solution"
Yulia Pushkar, Oleg Ayzatuln, Dietmar Stehlik *Applied Magnetic Resonance* 2005, V. 28, 195-211
88. "Asymmetric hydrogen-bonding of the quinone cofactor in Photosystem I probed by ¹³C labeled naphthoquinones"
Yulia Pushkar, Herbert Zimmermann, John H. Golbeck, Dietmar Stehlik *Journal of Physical Chemistry B* 2004, 108 (27) 9439-9448.

This paper was featured on the journal cover.
89. "An EPR/ENDOR study of the asymmetric hydrogen bond between the quinone electron acceptor and the protein backbone in Photosystem I"
Yulia Pushkar, Dietmar Stehlik, Maurice van Gastel, Wolfgang Lubitz *Journal of Molecular Structure* 2004, V. 700, 1-3, 233-241.
90. "Evidence for Asymmetric Electron Transfer in Cyanobacterial Photosystem I: Analysis of a Methionine to Leucine Mutation of the Ligand to the Primary Electron Acceptor A₀"
Wu Xu, Parag Chitnis, Alfia Valieva, Art van der Est, Yulia Pushkar, Dietmar Stehlik, Rachel Cohen, Gaozhong Shen, and John H. Golbeck *Biochemistry* 2004, 43(16); 4741-4754.
91. "Paramagnetic complexes of anthraquinone on the surface of Al₂O₃ and ZrO₂ according to the 3-mm wave band EPR spectra"
Fionov A.V., Pushkar Y., Lunina E.V. *Russian Journal of Physical Chemistry* 2004, 78(9), 1408-1412.
92. "Reactivity of palladium(II) methyl complexes towards CO₂: formation of carbonate complexes"
Yulia Pushkar, Ola F. Wendt *Inorganica Chimica Acta* 2004, 357, 1295-1298.

93. "Interpretation of multifrequency transient EPR spectra of the $P_{700}^+A_0Q_K^-$ state in Photosystem I complexes with a sequential correlated radical pair model: wild type versus A0 mutants"
Kev M. Salikhov, Yulia Pushkar, John H. Golbeck, Dietmar Stehlik *Applied Magnetic Resonance* 2003, 24, 467-482.
94. "Electron Transfer in Cyanobacterial Photosystem I. I. Physiological and Spectral Characterization of Site-Directed Mutants in a Putative Electron Transfer Pathway from A_0 through A_1 to F_X "
Wu Xu, Parag Chitnis, Yulia Pushkar, Christian Teutloff, Stephan G. Zech, Robert Bittl, Dietmar Stehlik, Alfia Valieva, Art van der Est, Boris Zybailov, Gaozhong Shen, and John H. Golbeck *Journal of Biological Chemistry* 2003, 278, 30, 27864-27875.
95. "Electron Transfer in Cyanobacterial Photosystem I. II. Determination of Forward Electron Transfer Rates of Site-Directed Mutants in a Putative Electron Transfer Pathway from A_0 through A_1 to F_X "
Klaus Brettel, Parag R. Chitnis, Art van der Est, John H. Golbeck, Mariana Guergova-Kuras, Yulia Pushkar, Gaozhong Shen, Dietmar Stehlik, Alfia Valieva, Wu Xu, Stephan G. Zech, Boris Zybailov *Journal of Biological Chemistry* 2003, 278, 30, 27876-27887.
96. "Orientation and protein-cofactor interactions of monosubstituted n-alkyl naphthoquinones in the A_1 binding site of Photosystem I"
Yulia Pushkar, Stephan G. Zech, Sarah Brown, Art van der Est, Herbert Zimmermann, Dietmar Stehlik *Journal of Physical Chemistry B* 2002, 106(46); 12052-12058.
97. "Structure and Lewis acid properties of Gallia-alumina catalysts"
Y. Pushkar, O.O. Parenago, A. Sinitsky, A.N. Kharlanov, E.V. Lunina *Applied Surface Science* 2000, 67, p. 69-78.
98. "Coordination of nitroxyl radical probes to the Lewis acid sites on the surface of gallium oxide: a quantum-chemical analysis"
A.M. Tokmachev, Y. Pushkar, E.V. Lunina, N.D. Chuvylkin *Russian Chemical Bulletin* 2000, 49, 6, p. 991-996.
99. "Paramagnetic complexes of probe molecules with electron-accepting sites on the surface of $M_2O_3-ZrO_2$ (M=Al, Ga)."
Y. Pushkar, O.O. Parenago, A.V. Fionov, E.V. Lunina *Colloids and Surface A: Physicochemical and Engineering Aspects* 1999, 158, 1-2 p. 179-187.
100. "Role of the crystalline structure in the formation of Lewis acid sites at the surface of gallium oxide"
O.O. Parenago, Y. Pushkar, A.O. Turakulova, G.P. Murav'eva, E.V. Lunina *Kinetic and Catalysis* 1998, 39, 2 268-273.