CURRICULUM VITAE

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Education

1981-1986: Moscow State University, Chemistry Department, Moscow, Russia; Major in Physical Chemistry, Quantum and Computational Chemistry; Minor in Theoretical Physics.

1986-1989: Postgraduate study at the Karpov Institute of Physical Chemistry, Moscow, Russia. Chemical Physics and Theory of Elementary Processes; Quantum Chemistry and Solid State Physics (Electronic Structure of Transition Metal Compounds); Quantum Statistical Mechanics.

Academic degrees

June 20, 1986: M.Sc. in Chemistry, Moscow State University, Chemistry Department, Moscow, Russia. M.Sc. Thesis: "The system of parameters of the effective Hamiltonian for the Titanium atom and its ions". Speciality: Theoretical and computational chemistry.

May 8, 1992: Ph.D. in Physics and Mathematics, Karpov Institute of Physical Chemistry, Moscow, Russia. Ph.D. Thesis: "Electronic Structure of Transition Metal Complexes". Speciality: Chemical physics and theory of elementary processes.

Awards

- International Science Foundation Research Award, 1993.
- Alexander von Humboldt Research Fellowship, 1994–1996.

Professional Experience

Since June 2018: Research Scientist, Department of Chemistry, Yale University, New Haven, CT, USA.

February 2013 – May 2018: Research Assistant Professor, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL, USA.

August 2002 – January 2013: Research Assistant Professor, Department of Chemistry, The Pennsylvania State University, University Park, PA, USA.

July 2000 – August 2002: Research Associate in the group of Professor Gregory A. Voth, Department of Chemistry and Henry Eyring Center for Theoretical Chemistry, University of Utah, Salt Lake City, UT, USA.

April 1998 – June 2000: Research Associate in the group of Professor Sharon Hammes-Schiffer, Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN, USA.

1996–1998: Senior Research Associate at the Quantum Chemistry and Statistical Physics Laboratory directed by Professor M. V. Basilevsky, Karpov Institute of Physical Chemistry, Moscow, Russian Federation.

1994–1996: Alexander von Humboldt Research Fellow in the group of Professor Dr. Karl Jug, Theoretische Chemie, University of Hannover, Hannover, Germany.

1992–1994: Research Associate at the Quantum Chemistry and Statistical Physics Laboratory directed by Professor M. V. Basilevsky, Karpov Institute of Physical Chemistry, Moscow, Russia.

Research Experience

- Quantum calculations of atomic spectra of transition metal atoms and ions (M.Sc. Thesis).
- Development of a new quantum-chemical method for calculations of the electronic structure, optical spectra and magnetic properties of transition metal complexes (Ph.D. Thesis).[36,46,87,89,90,93–95]
- Magnetic properties of low-dimensional materials (conjugated polymers and charge-transfer molecular crystals).
- Large scale *ab initio* and semiempirical quantum chemical calculations of the chemical reactions (potential energy surfaces: stationary points and reaction paths) of organic molecules and proton transfer systems.
- Dielectric continuum theory of equilibrium and non-equilibrium solvation in polar solvents.[33,41,83]
- Dynamical theory of complex charge transfer reactions (electron transfer, proton transfer, proton-coupled electron transfer) in condensed phases.[34,38,44,47,49,50,53,65,70,75,77,82,86,88]
- Analysis of quantum-classical approximations for the dynamics of non-adiabatic transitions in dissipative systems.[44,47,50,53,60,61,86]
- Modeling of hydrogen tunneling reactions in molecular crystals at low temperatures.[80]
- Quantum and classical molecular dynamics simulations of chemical reactions in solution and in biological systems.[38,44,47,49–53,55,57,58,60,61,67,69,72]
- Development of the Empirical Valence Bond (EVB) methodology for molecular dynamics simulations of biological systems.[69,79]
- Theory of proton-coupled electron transfer processes in solution and at metal and semiconductor interfaces.[15,28,30,35,40,49,50,53,57,60,63–65,67,70,75–78,81,83]
- Theoretical studies of proton-coupled electron transfer reactions in biological systems.[13,15,19,23,28,29,32,37,43,51,55,63,67,78]
- Quantum-classical surface hopping nonadiabatic dynamics of photoinduced proton-coupled electron transfer processes in complex environments.[34,38,44,47,50,52,53]
- Theory of interfacial proton-coupled electron transfer processes in electrochemical environment.[20,21,25–27,33,41,48,54,65,66]
- Artificial neural networks in quantum mechanics and quantum dynamics.[17,18]
- Electronic Structure and Nonadiabatic Quantum Dynamics Simulations and Algorithms for Quantum Computing.[1]
- Classical and Quantum Machine Learning Models for applications in Drug Design

Teaching Experience

- Course "Introduction to Theoretical Physics", College of Information Technologies, Moscow, 1992/1993.
- Undergraduate level course "Applied Quantum Chemistry: Potential Energy Surfaces for chemical reactions in the gas phase and in condensed medium", Higher Chemical College of Russian Academy of Sciences, Moscow, Fall Semester 1997.
- Undergraduate level course "Introduction to the theory of charge transfer reactions in condensed phases", Higher Chemical College of Russian Academy of Sciences, Moscow, Spring Semester 1998.
- Teaching assistance: Quantum Mechanics for graduate students, Department of Chemistry, The Pennsylvania State University, University Park, Pennsylvania, USA.
- Lectures on Molecular Dynamics Simulations of Molecular Systems (substitute lecturer, Chem 464: Chemical Kinetics and Dynamics, advanced undergraduate course), Department of Chemistry, Pennsylvania State University, Fall Semester 2009, 2010, 2011.
- Co-advised 14 graduate students and 12 postdoctoral associates

Computer Experience

- Programming languages: Fortran 77/90/2003/2008, C, C++, Python, Wolfram Mathematica.

  Coding projects:

  - EHCF - Quantum-chemistry package for calculation of electronic structure and electronic spectra of transition metal compounds (FORTRAN 77)
  - EHCF-SINDO1 - Incorporation of the EHCF method into the semiempirical quantum chemistry package SINDO1 (FORTRAN 77/C)
  - DLEVB - Multi-state EVB algorithm for molecular dynamics simulations of proton transfer processes in solution and biological environments (based on the DL_POLY package, FORTRAN 90/C
  - PCET - software package for calculations of rates and isotope effects of PCET reactions in solution and biological environments (FORTRAN 90/C)
  - DLPROTEIN_EVB - incorporation of the EVB methodology and force fields into the molecular dynamics simulation package DLPROTEIN (FORTRAN 90/C)
  - mathPCET - Wolfram Mathematica package containing functions and subroutines for the calculation of rates and kinetic isotope effects of PCET reactions
- Other programming and script languages: UNIX shells (bash, csh), awk, Perl.
- Expert in Wolfram Mathematica.
- Operating Systems: Microsoft Windows; Mac OS X; IBM AIX, HP-UX, Sun Solaris, SGI Irix, Linux.
- System and network administration of UNIX Clusters (IBM AIX, HP-UX, SGI Irix, Linux); administration and maintenance of Beowulf computer clusters.
- Parallel programming for shared memory and distributed memory computer clusters (OpenMP, MPI).
- OpenACC programming for GPUs.
- Web programming: Javascript, CGI, JSP, webMathematica

  Web development projects

  - webPCET - https://webpcet.chem.yale.edu - Java application server powered by Wolfram webMathematica: interactive simulations of proton-coupled electron transfer reactions on the web (Java Server Pages (JSP) servlets technology, JDBC, Java, Mathematica, Javascript, Perl, PHP, MySQL databases).

- Databases: MySQL, MongoDB.
- Machine Learning libraries and toolkits: PyTorch, TensorFlow.
- Molecular graphics and molecular modeling programs: Molden, GOpenMol, JMol, VMD, Maestro (Schrodinger LLC), and others.
- Quantum Chemistry Packages: Gaussian, GAMESS US, Q-Chem, MOLPRO, MOLCAS, Jaguar (Schrödinger LLC).
- Solid State Electronic Structure packages: Quantum Espresso, ABINIT, VASP, CP2K.
- Molecular Dynamics Programs: DL_POLY, CHARMM, GROMOS, AMBER, TINKER, GROMACS, NAMD, Desmond (D. E. Shaw Research).

Invited Talks and Seminars

1. University of Hannover Physical Chemistry Seminar, Hannover, Germany, May 16, 1996 (talk): "Effective Hamiltonian - Crysral Field approach on the INDO level: SINDO1 adaptation and applications to optical and Moessbauer spectra of large transition metal complexes".
2. INTAS Workshop on Dynamics of Proton Transfer Reactions in Polar Medium, Nancy, France, January 21-22, 1998 (talk): "Models of PT reactions in polar solvents. Non-adiabatic transitions between electron-proton states"
3. Midwest Theoretical Chemistry Conference, Notre Dame, Indiana, May 20-22, 1999 (talk): "Multistate continuum theory for proton-coupled electron transfer reactions in polar medium"
4. Pennsylvania State University Physical Chemistry Seminar, University Park, Pennsylvania, September 20, 2002 (talk): "Direct calculation of pKa for amino acid residues by means of molecular dynamics simulations: Implications for enzyme catalysis"
5. Quantum Atomic and Molecular Tunneling in Solids, University of Florida, Gainesville, Florida, June 22-25, 2003 (talk): "Recent advances and applications of the theory of proton-coupled electron transfer reactions in condensed phases"
6. Seminar of the New York section of the American Chemical Society, Syracuse University, Syracuse, November 14, 2004: "Theoretical models for complex charge transfer reactions in solution and biological environment"
7. DARPA Protein Design Processes (PDP) Program Workshop, Seattle, Washington, September 7-8, 2005: "Quantum-chemical probes in protein design algorithms".
8. DARPA Protein Design Processes (PDP) Program Workshop, Los Angeles, California, January 24-25, 2007: "Ranking protein designs: EVB approach to estimating the transition state structures".
9. Biological Physics Seminar at the Center for Biological Physics, Arizona State University, Tempe, Arizona, March 28, 2007: "Non-adiabatic Hydrogen Tunneling in Enzymes: Rates and Isotope Effects".
10. DARPA Protein Design Processes (PDP) Program Workshop, Santa Fe, New Mexico, June 13-14, 2007: "EVB approach for ranking protein designs: catalytic antibodies for Kemp elimination reaction".
11. American Chemical Society 234$^{\text{th}}$ National Meeting, Boston, Massachussets, August 19-23, 2007: "Extended Spin-Boson model for nonadiabatic hydrogen tunneling in the condensed phase".

12. Brookhaven National Laboratory, Center for Functional Nanomaterials, Computational Materials Theory Meeting; Upton, NY, January 12, 2010: "Interfacial Proton-Coupled Electron Transfer: Electrochemical and Photoinduced Processes".

13. 217th Electrochemical Society Meeting - Vancouver, Canada, April 26, 2010: "Theoretical Studies of Interfacial Proton-Coupled Electron Transfer Reactions at Metal Electrodes".

14. International Lorentz Center Workshop on Modeling Natural and Artificial Photosynthesis, March 7-11, 2011, Leiden, Niederlands. Title of the talk: "Theoretical Modeling of Ultrafast Photoinduced Proton- Coupled Electron Transfer".

15. 16th ETSF Workshop on Electronic Excitations: Bridging theory and experiment, 27-30 September 2011, Turin, Italy. Title of the talk: "Theoretical studies of ultrafast photoinduced proton-coupled electron transfer reactions".

16. International Workshop on New Materials For Renewable Energy, 17-21 October 2011, The Abdus Salam International Center for Theoretical Physics, Miramare, Trieste, Italy. Talk 1: "Theoretical Modeling of Proton-Coupled Electron Transfer Reactions in Energy Related Materials"; Talk 2: "Non-equilibrium dynamics of photoinduced proton-coupled electron transfer".

17. American Physical Society March Meeting, 3-7 March 2014, Denver, Colorado, USA: "Nonadiabatic dynamics of photoinduced proton-coupled electron transfer processes in solution".

18. GDCh-Festkolloquium zum 75. Geburtstag von Prof. Dr. Karl Jug. Leibniz Universität Hannover, October 25, 2014, Hannover, Germany: "Probing Nonadiabaticity in Proton-Coupled Electron Transfer".

19. International Workshop on Computational Electrochemistry (IWCE 2018), July 9-12, 2018, Aalto University, Helsinki, Finland: "Modeling Electrochemical Proton-Coupled Electron Transfer Reactions at Metal Electrodes: Spanning Adiabatic and Nonadiabatic Regimes".

Publications (in reverse chronological order)

1. Dutta, R., Vu, N. P., Xu, C., Cabral, D. G. A., Lyu, N., Soudackov, A. V., Dan, X., Li, H., Wang, C. & Batista, V. S. Simulating Electronic Structure on Bosonic Quantum Computers. *Journal of Chemical Theory and Computation.* doi:10.1021/acs.jctc.4c01400. eprint: 2404.10222 (2025).

2. Zhong, J., Zhu, Q., Soudackov, A. V. & Hammes-Schiffer, S. Hydrogen Tunneling and Conformational Motions in Nonadiabatic Proton-Coupled Electron Transfer between Interfacial Tyrosines in Ribonucleotide Reductase. *Journal of the American Chemical Society* **147,** 4459–4468. doi:10.1021/jacs.4c15756 (2025).

3. Kessinger, M. C., Xu, J., Cui, K., Loague, Q., Soudackov, A. V., Hammes-Schiffer, S. & Meyer, G. J. Direct Evidence for a Sequential Electron Transfer-Proton Transfer Mechanism in the PCET Reduction of a Metal Hydroxide Catalyst. *Journal of the American Chemical Society* **146,** 1742–1747. doi:10.1021/jacs.3c10742 (2024).

4. Lewis, N. B., Bisbey, R. P., Westendorff, K. S., Soudackov, A. V. & Surendranath, Y. A molecular-level mechanistic framework for interfacial proton-coupled electron transfer kinetics. *Nature Chemistry,* 1–10. doi:10.1038/s41557-023-01400-0 (2024).

5. Warburton, R. E., Soudackov, A. V. & Hammes-Schiffer, S. Interfacial Proton-Coupled Electron Transfer via Localized Trap States on Metal Oxide Surfaces. *The Journal of Physical Chemistry C.* doi:10.1021/acs.jpcc.4c00458 (2024).

6. Zhong, J., Soudackov, A. V. & Hammes-Schiffer, S. Probing Nonadiabaticity of Proton-Coupled Electron Transfer in Ribonucleotide Reductase. *The Journal of Physical Chemistry Letters* **15,** 1686–1693. doi:10.1021/acs.jpclett.3c03552 (2024).

7. Cui, K., Soudackov, A. V., Kessinger, M. C., Xu, J., Meyer, G. J. & Hammes-Schiffer, S. General Kinetic Model for pH Dependence of Proton-Coupled Electron Transfer: Application to an Electrochemical Water Oxidation System. *Journal of the American Chemical Society* **145,** 19321–19332. doi:10.1021/jacs.3c05535 (2023).
8. Konstantinovsky, D., Perets, E. A., Santiago, T., Olesen, K., Wang, Z., Soudackov, A. V., Yan, E. C. & Hammes-Schiffer, S. Design of an Electrostatic Frequency Map for the NH Stretch of the Protein Backbone and Application to Chiral Sum Frequency Generation Spectroscopy. *Journal of Physical Chemistry B* **127,** 2418–2429. doi:10.1021/acs.jpcb.3c00217 (2023).
9. Rousseau, B. J. G., Soudackov, A. V., Tuttle, R. R., Reynolds, M. M., Finke, R. G. & Hammes-Schiffer, S. Computational Insights into the Mechanism of Nitric Oxide Generation from S-Nitrosoglutathione Catalyzed by a Copper Metal-Organic Framework. *Journal of the American Chemical Society* **145,** 10285–10294. doi:10.1021/jacs.3c01569 (2023).
10. Secor, M., Soudackov, A. V. & Hammes-Schiffer, S. Density Matrix-Based Features as Descriptors for Oxygen Reduction and Evolution Catalysts. *The Journal of Physical Chemistry C* **127,** 15246–15256. doi:10.1021/acs.jpcc.3c03392 (2023).
11. Yang, Y., Agarwal, R. G., Hutchison, P., Rizo, R., Soudackov, A. V., Lu, X., Herrero, E., Feliu, J. M., Hammes-Schiffer, S., Mayer, J. M. & Abruña, H. D. Inverse kinetic isotope effects in the oxygen reduction reaction at platinum single crystals. *Nature Chemistry* **15,** 271–277. doi:10.1038/s41557-022-01084-y (2023).
12. Kessinger, M., Soudackov, A. V., Schneider, J., Bangle, R. E., Hammes-Schiffer, S. & Meyer, G. J. Reorganization Energies for Interfacial Proton-Coupled Electron Transfer to a Water Oxidation Catalyst. *Journal of the American Chemical Society* **144,** 20514–20524. doi:10.1021/jacs.2c09672 (2022).
13. Reinhardt, C. R., Konstantinovsky, D., Soudackov, A. V. & Hammes-Schiffer, S. Kinetic model for reversible radical transfer in ribonucleotide reductase. *Proceedings of the National Academy of Sciences* **119,** e2202022119. doi:10.1073/pnas.2202022119 (2022).
14. Yang, Y., Peltier, C. R., Zeng, R., Schimmenti, R., Li, Q., Huang, X., Yan, Z., Potsi, G., Selhorst, R., Lu, X., Xu, W., Tader, M., Soudackov, A. V., Zhang, H., Krumov, M., Murray, E., Xu, P., Hitt, J., Xu, L., Ko, H.-Y., Ernst, B. G., Bundschu, C., Luo, A., Markovich, D., Hu, M., He, C., Wang, H., Fang, J., DiStasio, R. A., Kourkoutis, L. F., Singer, A., Noonan, K. J. T., Xiao, L., Zhuang, L., Pivovar, B. S., Zelenay, P., Herrero, E., Feliu, J. M., Suntivich, J., Giannelis, E. P., Hammes-Schiffer, S., Arias, T., Mavrikakis, M., Mallouk, T. E., Brock, J. D., Muller, D. A., DiSalvo, F. J., Coates, G. W. & Abruña, H. D. Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies. *Chemical Reviews* **122,** 6117–6321. doi:10.1021/acs.chemrev.1c00331 (2022).
15. Barragan, A. M., Soudackov, A. V., Luthey-Schulten, Z., Hammes-Schiffer, S., Schulten, K. & Solov'yov, I. A. Theoretical Description of the Primary Proton-Coupled Electron Transfer Reaction in the Cytochrome bc_1 Complex. *Journal of the American Chemical Society* **143,** 715–723. doi:10.1021/jacs.0c07799 (2021).
16. Hutchison, P., Warburton, R. E., Soudackov, A. V. & Hammes-Schiffer, S. Multicapacitor Approach to Interfacial Proton-Coupled Electron Transfer Thermodynamics at Constant Potential. *Journal of Physical Chemistry C* **125,** 21891–21901. doi:10.1021/acs.jpcc.1c04464 (2021).
17. Secor, M., Soudackov, A. V. & Hammes-Schiffer, S. Artificial Neural Networks as Mappings between Proton Potentials, Wave Functions, Densities, and Energy Levels. *Journal of Physical Chemistry Letters* **12,** 2206–2212. doi:10.1021/acs.jpclett.1c00229 (2021).
18. Secor, M., Soudackov, A. V. & Hammes-Schiffer, S. Artificial Neural Networks as Propagators in Quantum Dynamics. *Journal of Physical Chemistry Letters* **12,** 10654–10662. doi:10.1021/acs.jpclett.1c03117 (2021).
19. Veenis, A. J., Li, P., Soudackov, A. V., Hammes-Schiffer, S. & Bevilacqua, P. C. Investigation of the pK_a of the Nucleophilic O2′ of the Hairpin Ribozyme. *Journal of Physical Chemistry B* **125,** 11869–11883. doi:10.1021/acs.jpcb.1c06546 (2021).

20. Warburton, R. E., Soudackov, A. V. & Hammes-Schiffer, S. Theoretical Modeling of Electrochemical Proton-Coupled Electron Transfer. *Chemical Reviews* **122,** 10599–10650. doi:10.1021/acs.chemrev.1c00929 (2021).

21. Lam, Y.-C., Soudackov, A. V. & Hammes-Schiffer, S. Theory of Electrochemical Proton-Coupled Electron Transfer in Diabatic Vibronic Representation: Application to Proton Discharge on Metal Electrodes in Alkaline Solution. English. *Journal of Physical Chemistry C* **124,** 27309–27322. doi:10.1021/acs.jpcc.0c08096 (2020).

22. Li, P., Soudackov, A. V., Koronkiewicz, B., Mayer, J. M. & Hammes-Schiffer, S. Theoretical Study of Shallow Distance Dependence of Proton-Coupled Electron Transfer in Oligoproline Peptides. *Journal of the American Chemical Society* **142,** 13795–13804. doi:10.1021/jacs.0c04716 (2020).

23. Barragan, A. M., Soudackov, A. V., Luthey-Schulten, Z., Schulten, K., Hammes-Schiffer, S. & Solov'yov, I. Unveiling the Rate-Limiting Step of the Bc1 Complex Reaction Mechanism. English. *Biophysical Journal* **116,** 419a. doi:10.1016/j.bpj.2018.11.2257 (2019).

24. Goldsmith, Z. K., Soudackov, A. V. & Hammes-Schiffer, S. Theoretical analysis of the inverted region in photoinduced proton-coupled electron transfer. English. *Faraday Discussions* **216,** 363–378. doi:10.1039/c8fd00240a (2019).

25. Lam, Y.-C., Soudackov, A. V., Goldsmith, Z. K. & Hammes-Schiffer, S. Theory of Proton Discharge on Metal Electrodes: Electronically Adiabatic Model. English. *Journal of Physical Chemistry C* **123,** 12335–12345. doi:10.1021/acs.jpcc.9b02148 (2019).

26. Lam, Y.-C., Soudackov, A. V. & Hammes-Schiffer, S. Kinetics of Proton Discharge on Metal Electrodes: Effects of Vibrational Nonadiabaticity and Solvent Dynamics. English. *Journal of Physical Chemistry Letters* **10,** 5312–5317. doi:10.1021/acs.jpclett.9b01984 (2019).

27. Goldsmith, Z. K., Lam, Y. C., Soudackov, A. V. & Hammes-Schiffer, S. Proton Discharge on a Gold Electrode from Triethylammonium in Acetonitrile: Theoretical Modeling of Potential-Dependent Kinetic Isotope Effects. English. *Journal of the American Chemical Society* **141,** 1084–1090. doi:10.1021/jacs.8b11826 (2018).

28. Li, P., Soudackov, A. V. & Hammes-Schiffer, S. Fundamental Insights into Proton-Coupled Electron Transfer in Soybean Lipoxygenase from Quantum Mechanical/Molecular Mechanical Free Energy Simulations. English. *Journal of the American Chemical Society* **140,** 3068–3076. doi:10.1021/jacs.7b13642 (2018).

29. Li, P., Soudackov, A. V. & Hammes-Schiffer, S. Impact of Mutations on the Binding Pocket of Soybean Lipoxygenase: Implications for Proton-Coupled Electron Transfer. English. *Journal of Physical Chemistry Letters* **9,** 6444–6449. doi:10.1021/acs.jpclett.8b02945 (2018).

30. Ghosh, S., Castillo-Lora, J., Soudackov, A. V., Mayer, J. M. & Hammes-Schiffer, S. Theoretical Insights into Proton-Coupled Electron Transfer from a Photoreduced ZnO Nanocrystal to an Organic Radical. English. *Nano Letters* **17,** 5762–5767. doi:10.1021/acs.nanolett.7b02642 (2017).

31. Ghosh, S., Soudackov, A. V. & Hammes-Schiffer, S. Role of Proton Diffusion in the Nonexponential Kinetics of Proton-Coupled Electron Transfer from Photoreduced ZnO Nanocrystals. English. *ACS Nano* **11,** 10295–10302. doi:10.1021/acsnano.7b05009 (2017).

32. Hu, S., Soudackov, A. V., Hammes-Schiffer, S. & Klinman, J. P. Enhanced Rigidification within a Double Mutant of Soybean Lipoxygenase Provides Experimental Support for Vibronically Nonadiabatic Proton-Coupled Electron Transfer Models. English. *ACS Catalysis* **7,** 3569–3574. doi:10.1021/acscatal.7b00688 (2017).

33. Ghosh, S., Soudackov, A. V. & Hammes-Schiffer, S. Electrochemical Electron Transfer and Proton-Coupled Electron Transfer: Effects of Double Layer and Ionic Environment on Solvent Reorganization Energies. English. *Journal of Chemical Theory and Computation* **12,** 2917–2925. doi:10.1021/acs.jctc.6b00233 (2016).

34. Goyal, P., Schwerdtfeger, C. A., Soudackov, A. V. & Hammes-Schiffer, S. Proton Quantization and Vibrational Relaxation in Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer in a Solvated Phenol-Amine Complex. English. *Journal of Physical Chemistry B* **120,** 2407–2417. doi:10.1021/acs.jpcb.5b12015 (2016).

35. Soudackov, A. V. & Hammes-Schiffer, S. Proton-coupled electron transfer reactions: analytical rate constants and case study of kinetic isotope effects in lipoxygenase. English. *Faraday Discussions* **195,** 171–189. doi:10.1039/c6fd00122j (2016).

36. Tchougréeff, A. L., Soudackov, A. V., van Leusen, J., Kögerler, P., Becker, K. & Dronskowski, R. Effective hamiltonian crystal field: Present status and applications to iron compounds. English. *International Journal of Quantum Chemistry* **116** (ed Tchougréeff, A. L.) 282–294. doi:10.1002/qua.25016 (2016).

37. Yu, T., Soudackov, A. V. & Hammes-Schiffer, S. Computational Insights into Five- versus Six-Coordinate Iron Center in Ferrous Soybean Lipoxygenase. English. *Journal of Physical Chemistry Letters* **7,** 3429–3433. doi:10.1021/acs.jpclett.6b01626 (2016).

38. Goyal, P., Schwerdtfeger, C. A., Soudackov, A. V. & Hammes-Schiffer, S. Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer in a Solvated Phenol–Amine Complex. English. *Journal of Physical Chemistry B* **119,** 2758–2768. doi:10.1021/jp5126969 (2015).

39. Harshan, A. K., Yu, T., Soudackov, A. V. & Hammes-Schiffer, S. Dependence of Vibronic Coupling on Molecular Geometry and Environment: Bridging Hydrogen Atom Transfer and Electron–Proton Transfer. English. *Journal of the American Chemical Society* **137,** 13545–13555. doi:10.1021/jacs.5b07327 (2015).

40. Soudackov, A. V. & Hammes-Schiffer, S. Nonadiabatic rate constants for proton transfer and proton-coupled electron transfer reactions in solution: Effects of quadratic term in the vibronic coupling expansion. English. *Journal of Chemical Physics* **143,** 194101. doi:10.1063/1.4935045 (2015).

41. Ghosh, S., Horvath, S., Soudackov, A. V. & Hammes-Schiffer, S. Electrochemical Solvent Reorganization Energies in the Framework of the Polarizable Continuum Model. English. *Journal of Chemical Theory and Computation* **10,** 2091–2102. doi:10.1021/ct500051e (2014).

42. Herlitschke, M., Tchougréeff, A. L., Soudackov, A. V., Klobes, B., Stork, L., Dronskowski, R. & Hermann, R. P. Magnetism and lattice dynamics of FeNCN compared to FeO. English. *New Journal of Chemistry* **38,** 4670–4677. doi:10.1039/c4nj00097h (2014).

43. Hu, S., Sharma, S. C., Scouras, A. D., Soudackov, A. V., Carr, C. A. M., Hammes-Schiffer, S., Alber, T. & Klinman, J. P. Extremely Elevated Room-Temperature Kinetic Isotope Effects Quantify the Critical Role of Barrier Width in Enzymatic C − H Activation. English. *Journal of the American Chemical Society* **136,** 8157–8160. doi:10.1021/ja502726s (2014).

44. Schwerdtfeger, C. A., Soudackov, A. V. & Hammes-Schiffer, S. Nonadiabatic dynamics of electron transfer in solution: Explicit and implicit solvent treatments that include multiple relaxation time scales. English. *Journal of Chemical Physics* **140,** 034113. doi:10.1063/1.4855295 (2014).

45. Soudackov, A. V. & Hammes-Schiffer, S. Probing Nonadiabaticity in the Proton-Coupled Electron Transfer Reaction Catalyzed by Soybean Lipoxygenase. English. *Journal of Physical Chemistry Letters* **5,** 3274–3278. doi:10.1021/jz501655v (2014).

46. Tchougréeff, A. L. & Soudackov, A. V. Effective Hamiltonian crystal fields: Present status and applicability to magnetic interactions in polynuclear transition metal complexes. English. *Russian Journal of Physical Chemistry A* **88,** 1904–1913. doi:10.1134/s0036024414110053 (2014).

47. Auer, B., Soudackov, A. V. & Hammes-Schiffer, S. Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer: Comparison of Explicit and Implicit Solvent Simulations. English. *Journal of Physical Chemistry B* **116,** 7695–7708. doi:10.1021/jp3031682 (2012).

48. Horvath, S., Fernandez, L. E., Soudackov, A. V. & Hammes-Schiffer, S. Insights into proton-coupled electron transfer mechanisms of electrocatalytic H2 oxidation and production. English. *Proceedings of the National Academy of Sciences* **109,** 15663–15668. doi:10.1073/pnas.1118333109 (2012).

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