Tao Yu

Department of Chemistry University of North Dakota tao.yu.1@und.edu 701-777-4908
Research Group Website: https://comchemyu.github.io/und.research.github.io/
Google Scholar: https://scholar.google.com/citations?user=28k5ExIAAAAJ&hl=en

EDUCATION

07/2012 Ph.D. in Chemistry, University of Minnesota
07/2007 M.Sc. in Chemistry, Fudan University in Shanghai
07/2004 B.Sc. in Chemistry, Fudan University in Shanghai

RESEARCH INTERESTS

Theoretical/Computational Biophysics/Biochemistry
Theoretical/Computational Materials Chemistry

PROFESSIONAL EXPERIENCE

08/2019 – Present	Assistant Professor	University of North Dakota
08/2016 - 07/2019	Assistant Professor	Tennessee Technological University
09/2014 - 07/2016	Postdoctoral	University of Illinois at Urbana-Champaign
08/2012 - 08/2014	Postdoctoral	Northwestern University

HONORS AND AWARDS

2019 DOE Visiting Faculty Program Fellowship
2018DOE Visiting Faculty Program Fellowship

Grants

1. NSF: Regulatory Functions of Intrinsically Disordered Electronegative Clusters (ENC) in RNA-Binding Proteins, Co-PI, $900,000, 08/2020-07/31/2024
2. NSF: RII Track-1: ND-ACES: New Discoveries in the Advanced Interface of Computation, Engineering, and Science, Computational Pillar Co-Lead, $3,061,410.00, 07/2020-06/30/2025

INVITED PRESENTATIONS

1. 05/2019 “A Fast Scheme to Calculate Electronic Couplings between Poly(3-Hexylthiophene) Units Using Diabatic Orbitals for Charge Transfer Dynamics Simulations”, SETCA
2. 02/2019 “Charge, Energy, Hydrogen, and Proton-Coupled Electron Transfer Reactions in Protein and Material Systems”, Oregon State University
3. 09/2017 “Enzyme-catalyzed hydride and proton-coupled electron transfer reactions. Self-assembly of peptide amphiphiles”, Middle Tennessee State University
4. 10/2016 “Enzyme-catalyzed hydride and proton-coupled electron transfer reactions. Self-assembly of peptide amphiphiles”, Molecular Biophysics Center at Oak Ridge National Lab
5. 3/2016 “Enzyme-catalyzed hydride and proton-coupled electron transfer reactions. Self-assembly of peptide amphiphiles”, Department of Chemistry, New York University
6. 11/2014 “Structure and dynamics of complex chemical systems”, Department of Chemistry, Brookhaven National Lab

7. 12/2013 "Computational approach to study structure and dynamics of complex chemical systems", Department of Chemistry, Clemson University

TEACHING EXPERIENCE

General Chemistry Lecture and Lab
Physical Chemistry Lecture and Lab
Advanced Molecular Modeling

CONFERENCE PRESENTATIONS

1. **T. Yu**, F. Fabunmi, J. Huang, J. Jakowsiki, and B. Sumpter, "Fast scheme to calculate electronic couplings between poly-3-hexylthiophene polymer units using diabatic orbitals for charge transfer dynamics simulations", Southeast Regional ACS Meeting, Augusta, GA, 2018.
2. **T. Yu** and A. Ridings **"**Self-assembly of AAT molecule and RNA delivery", 255th ACS National Meeting, New Orleans, LA, 2018.
3. **T. Yu** and A. Ridings, **"**Self-assembly of AAT nanotube and RNA delivery", Southeast Regional ACS Meeting, Charlotte, NC, 2017.
4. **T. Yu**, G. C. Schatz, and J. Licht "Mutation induced structure changes in histone proteins", 253rd ACS Meeting San Francesco, CA, 2017.
5. **T. Yu**, OS. Lee, and G. C. Schatz, "Studies of self-assembly mechanism of peptide amphiphiles and application of peptide-amphiphile nanofibers as photonic nanowires", Gordon Research Conference, Boston, 2014.
6. **T. Yu**, OS. Lee, and G. C. Schatz, "Studies of self-assembly mechanism of peptide amphiphiles and application of peptide-amphiphile nanofibers as photonic nanowires", Midwest Theoretical Chemistry Conference, IL, 2014.
7. **T. Yu**, J. Zheng, and D. G. Truhlar, "Multi-structural variational transition state theory. Kinetics of 1-4 hydrogen-shift isomerization of 1-pentyl radical", 242nd ACS National Meeting, Denver, CO, 2011.

PUBLICATION LIST

Google Scholar information

Citation: 1000, h-index: 17
https://scholar.google.com/citations?user=28k5ExIAAAAJ&hl=en

Tenure-Track Period:

2020

1. **T. Yu***, D. Lingerfelt*, J. Jakowski*, P. Ganesh, B. Sumpter *"Electron-Beam-Induced Molecular Plasmon Excitation and Energy Transfer in Silver Molecular Nanowires" submitted to J. Phys. Chem. C*
2. D. Lingerfelt*, **T. Yu***, A. Yoshimura, P. Ganesh, J. Jakowski, B. Sumpter *"Nonadiabatic Effects on Defect Diffusion in Silicon-Doped Nanographenes" submitted to Nano. Lett.*
3. B. He, X. Wang, L. Xia, Y. Guo, Y. Tang, Y. Zhao, Q. Hao, **T. Yu***, H. Liu*, Z. Su* Metal-organic framework-derived Fe-doped Co1.11Te2 embedded in nitrogen-doped carbon nanotube for water splitting. *ChemSusChem accepted*

4. W. Ren, K. Jiang, H. Deng, N. Lu, **T. Yu***, H. Guo*, P. Qian* Catalytic mechanism and product specificity of protein arginine methyltransferase PRMT7: A study from QM/MM molecular dynamics and free energy simulations. *J. Chem. Theory Comput.* 2020, 16, 8, 5301.
5. J. Chen, Q. Tao, J. Wu, M. Wang, Z. Su, Y. Qian, **T. Yu**, Y. Wang, X. Xue, H.-K. Liu A lysosome-targeted ruthenium(II) polypyridyl complex as photodynamic anticancer agent *J. Inorg. Biochem.* 2020, 210, 111132.

2019

6. R. A. Bennett, A. Bele, C. M. Will, E. C. Small, B. Nabet, R. Ghosh, A. T. Grzybowski, **T. Yu**, Q. Zhang, A. Riva, T. Lele, G. C. Schatz, A. J. Ruthenburg, J. Liphardt, and J. D. Licht, A mutation in the core of histone H2B represents a new class of oncogenic drivers, *Cancer Discov.* 2019, 10, 1438
7. **T. Yu***, F. Fabunmi, J. Huang, B. Sumpter, and J. Jakowski*, A fast scheme to calculate electronic couplings in P3HT polymer units using diabatic orbitals for charge transfer dynamics. *J. Comput. Chem.*, 2019, 40, 532.
8. W. H. Morris, J. D. Conner, L. Ngo, J. T.Wilson, W. Medawala, A. R. Brown, M. T. Stephens, F. Fabunmi, D. Cashman, E. C. Lisic, **T. Yu**, J. E. Deweese, and X. Jiang, Structural and metal ion effects on human topoisomerase IIα inhibition by α-(N)-heterocyclic thiosemicarbazones. *Chem. Res. Toxicol.* 2019, 32, 90.

2018

9. J. D. Marsee, A. Ridings, **T. Yu***, J. M. Miller*, Mycobacterium tuberculosis ClpC1 N-terminal domain is dispensable for adaptor protein-dependent allosteric regulation. *Int. J. Mol. Sci.* 2018, 19, 3651.

2017

10. J. Li, P. Zhang, Y. Xu, Z. Su, Y. Qian, S. Li, **T. Yu***, P. J Sadler*, H.-K. Liu*, A novel strategy to construct Janus metallamacrocycles with both a Ru-carene face and an imidazolium face. *Dalton Trans.* 2017, 46, 16205.
11. P. Wang, Y. Zhao, H. Zhang, **T. Yu**, Y. Zhang, Y. Tang, Effect of pyrazolium-derived compounds as templates in zeolite synthesis. RSC Adv., 2017, 7, 23272.
12. M. Horitani, A. R. Offenbacher, C. A. M. Carr, **T. Yu**, V. Hoeke, G. E. Cutsail III, S. Hammes-Schiffer, J. P. Klinman, B. M. Hoffman, 13C ENDOR spectroscopy of lipoxygenase–substrate complexes reveals the structural basis for C–H activation by tunneling. *J. Am. Chem. Soc.* 2017, 139, 1984.

Before Tenure-Track:

2016

13. **T. Yu**, A.V. Soudackov, and S. Hammes-Schiffer, Computational insights into five-versus six-coordinate iron center in ferrous soybean lipoxygenase. *J. Phys. Chem. Lett.* 2016, 7, 3429.
14. Z. Yu, F. Tantakitti, **T. Yu**, L. C. Palmer, G. C. Schatz, and S. I. Stupp, Simultaneous covalent and non-covalent polymerizations. *Science* 2016, 351, 497.
15. F. Tantakitti, J. Boekhoven, J. Li, E. Zhuang, R. Zandi, J. H. Ortony, C. J. Newcomb, L. C. Palmer, **T. Yu**, G. C. Schatz, Samuel I. Stupp, The energy landscapes of supramolecular systems determine their function. *Nat. Mater.* 2016, 15, 694.

2015

16. A. K. Harshan, **T. Yu (co-first author)**, A. V. Soudackov, and S. Hammes-Schiffer, Dependence of vibronic coupling on molecular geometry and environment: bridging hydrogen atom transfer and electron-proton transfer. *J. Am. Chem. Soc.*2015, 137, 13545.
17. F. Li, E. S. Burgie, **T.Yu***, A. Héroux, G. C. Schatz, R. D. Vierstra*, and A. M. Orville*, X-ray induced deprotonation of the Bilin chromophore in crystalline D. radiodurans phytochrome. *J. Am. Chem. Soc.* 2015, 137, 2792.

2014—2006

18. **T. Yu**, OS. Lee, and G. C Schatz, Molecular dynamics simulations and electronic excited state properties of a self-assembled peptide amphiphile nanofiber with metalloporphyrin arrays. *J. Phys. Chem. A* 2014, 118, 8553.
19. **T. Yu**, and G. C. Schatz, Free-Energy Landscape for peptide amphiphile self-assembly: stepwise versus continuous assembly mechanisms. *J. Phys. Chem. B* 2013, 117, 14059.
20. **T. Yu**, and G. C. Schatz, Free energy profile and mechanism of self-assembly of peptide amphiphiles based on a collective assembly coordinate. *J. Phys. Chem. B* 2013, 117, 9004.
21. **T. Yu**, OS. Lee, and G. C. Schatz, Steered molecular dynamics studies of the potential of mean force for peptide amphiphile self-assembly into cylindrical nanofibers. *J. Phys. Chem. A* 2013, 117, 7453.
22. **T. Yu**, J. M. Higashi, A. Cembran, J. Gao, and D. G. Truhlar, Concerted hydrogen atom and electron transfer mechanism for catalysis by lysine-specific demethylase. *J. Phys. Chem. B* 2013, 117, 8422. **(Cover Article)**
23. I. M. Alecu, J. Zheng, E. Papajak, **T. Yu**, and D. G. Truhlar, Biofuel combustion energetics and kinetics of hydrogen abstraction from carbon-1 in n-butanol by the hydroperoxyl radical calculated by coupled cluster and density functional theories and Multistructural variational transition-state theory with multidimensional tunneling. *J. Phys. Chem. A* 2012, 116, 12206.
24. X. F. Xu, **T. Yu**, E. Papajak, and D. G. Truhlar, Multistructural variational transition state theory: kinetics of the hydrogen abstraction from carbon-2 of 2-methyl-1-propanol by hydroperoxyl radical including all structures and torsional anharmonicity. *J. Phys, Chem. A* 2012, 116, 10480.
25. P. Seal, E. Papajak, **T. Yu**, and D. G. Truhlar, Statistical thermodynamics of 1-butanol, 2-methyl-1-propanol, and butanol. *J. Chem. Phys.* 2012, 136, 034306.
26. **T. Yu**, J. Zheng, and D. G. Truhlar, Multipath variational transition state theory: rate constant of the 1, 4-hydrogen shift isomerization of the 2-cyclohexylethyl radical. *J. Phys. Chem. A* 2012, 116, 297.
27. **T. Yu**, J. Zheng, and D. G. Truhlar, Statistical thermodynamics of the isomerization reaction between n-heptane and isoheptane. *Phys. Chem. Chem. Phys.* 2012, 14, 482.
28. **T. Yu**, J. Zheng, and D. G. Truhlar, Multi-structural variational transition state theory. Kinetics of the 1, 4-hydrogen shift isomerization of the pentyl radical with torsional anharmonicity. *Chem. Sci.* 2011, 11, 2199.
29. J. Zheng, **T. Yu**, and D. G. Truhlar, Multi-structural thermodynamics of C–H bond dissociation in hexane and isohexane yielding seven isomeric hexyl radicals. *Phys. Chem. Chem. Phys.* 2011, 13, 19318.
30. J. Zheng, **T. Yu**, E. Papajak, I, M. Alecu, S. L. Mielke, and D. G. Truhlar, Practical methods for including torsional anharmonicity in thermochemical calculations on complex molecules: The internal-coordinate multi-structural approximation. *Phys. Chem. Chem. Phys.* 2011, 13, 10885.

31. L. R. Masterson, **T. Yu**, L. Shi; Y. Wang, M. Gustavsson, M. M. Mueller, and G. Veglia, cAMP-dependent protein kinase A selects the excited state of the membrane substrate phospholamban. *J. Mol. Biol.* 2011, 412, 155.
32. L. R. Masterson, C.Y. Cheng, **T. Yu**, M. Tonelli, A. Kornev, S. S. Taylor, and G. Veglia, Dynamics connect substrate recognition to catalysis in protein kinase A. *Nat. Chem. Biol.* 2010, 6, 821.
33. L. R. Masterson, N. Bortone, **T. Yu**, K. N. Ha, E. C. Gaffarogullari, O. Nguyen, and G. Veglia, Expression and purification of isotopically labeled peptide inhibitors and substrates of cAMP-dependent protein kinase A for NMR analysis. *Prot. Expr. Pur.* 2009, 64, 231.
34. X. Q. Zhou, **T. Yu**, Y. H. Zhang, J. Kong, Y. Tang, J.-L. Marty, and B. Liu, Nanozeolite-assembled interface towards sensitive biosensing. *Electrochem. Commun.* 2007, 9, 1525.
35. **T. Yu**, Y. H. Zhang, J. H. Zhuang, B. Wang, B. H. Liu, Y. J. Kang, and Y. Tang, Controlled nanozeolite-assembled electrode: remarkable enzyme-immobilization ability and high sensitivity as biosensor. *Chem.-A Eur. J.* 2006, 12, 1137.
36. W. Shan, **T. Yu**, B. Wang, J. K. Hu, Y. H. Zhang, X. Y. Wang, and Y. Tang, Magnetically separable nanozeolites: promising candidates for bio-applications. *Chem. Mater.* 2006, 18, 3169.