Curriculum Vitae

PERSONAL DETATILS

Name: Feng Zhang

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EDUCATION

- Sept. 2006—Mar. 2010, Ph. D. in Theoretical Chemistry at Royal Institute of Technology, Stockholm, Sweden
  Thesis: *Theoretical Studies on Kinetics of Molecular Excited States* (Supervisor: Prof. Yi Luo)
- Sept. 2002—Jun.2008, Ph. D. in Physical Chemistry at Beijing Normal University, Beijing, China
  Thesis: *Theoretical Study of Non-adiabatic Effects in Photochemical Reactions* (Supervisor: Prof. Weihai Fang)
- Sept. 1998—Jun. 2002, Bachelor in Physical Education at FuYang Normal College, Fuyang, China

WORKING EXPERIENCE

- Jun. 2020 - present, Associate professor at the National Synchrotron Radiation Laboratory, University of Science and Technology of China, China
- Apr. 2012 – Jun. 2020, Associate professor at the National Synchrotron Radiation Laboratory, University of Science and Technology of China, China
- Mar. 2014 - Nov. 2014, Visiting Scholar, Argonne National Laboratory, U.S.A (working with Dr. Stephen J. Klippenstein)
- Aug. 2011 - May 2012, Post-doctoral researcher at the National Synchrotron Radiation Laboratory, University of Science and Technology of China, China (working with Prof. Fei Qi)
- Mar. 2010 - Jul. 2011, Post-doctoral researcher at the College of Environmental Science and Forestry, State University of New York, U.S.A (working with Prof. Theodore S. Dibble)

Funding:

- **Chemical kinetics of key excited species involved in hydrocarbon combustion, ¥580K, 2019.01-2022.12, PI**
  National Natural Science Foundation of China
- **Combustion kinetics of typical solid propellants, ¥250K, 2019.06-2020.12, PI**
  Xi'an Modern Chemistry Research Institute
- **Reaction mechanism of photochemical smog from volatile organic compounds, ¥700K of ¥1,950K, 2016.07-2020.06, co-PI**
  National Key Research and Development Program of China

- **The role of key excited species like OH* and O2(a1g) in hydrocarbon combustion, ¥648K, 2016.01-2018.12, PI**
  National Natural Science Foundation of China
- **Kinetic mechanism for low temperature oxidation of typical cyclic alkanes, ¥800K, 2014.01-2017.12, PI**
  National Natural Science Foundation of China
- **Formation mechanism of a typical combustion pollutant – naphthalene, ¥260K, 2014.01-2016.12, PI**
  National Natural Science Foundation of China

RESEARCH INTERESTS

1. High and low temperature combustion kinetics of hydrocarbons and oxygenated hydrocarbons, especially the OH&HO_2 chemistry and RO_2 chemistry; Combustion chemistry of nitrogen-containing energetic compounds.

2. Global uncertainty analysis of theoretically predicted rate constants; Reaction network analysis by graph theories.

3. Theoretical studies on photoionization behavior of organic molecules.

PUBLICATIONS

1. Hou, Q.; Niu, S.; Huang, C.; Wu, X.; Qu, W.; **Zhang, F.**, Decomposition of 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105): From thermodynamics to kinetics. *International Journal of Chemical Kinetics 53* (2), 242-249, (2021).
2. Huang, C.; Zhang, P; Wang, J.; Kang, S.; **Zhang, F.**; Law, C.; Yang, B. Determination of rate constants for a thermoneutral H-abstraction reaction: Allylic hydrogen abstraction from 1,5-hexadiene by allyl radical. Proceedings of the Combustion Institute. 10.1016/j.proci.2020.07.054. (2020).
3. Wu, X.; Huang, C.; Niu, S.; **Zhang, F**., New theoretical insights into the reaction kinetics of toluene and hydroxyl radicals. *Physical Chemistry Chemical Physics 22* (39), 22279-22288, (2020).
4. Huang, C.; Li, S.; Wang, J.; Yang, B.; **Zhang, F.**, Global uncertainty analysis for the RRKM/master equation modeling of a typical multi-well and multi-channel reaction system. *Combustion and Flame 216*, 62-71, (2020).
5. **Zhang, F.**; Huang, C.; Wu, X.; Binbin, X.; Shen, L. An insight into the reaction kinetics of CH3 + O2(a1Δg) and its enhancement effect on methane ignition. Proceedings of the Combustion Institute. 1-8. 10.1016/j.proci.2020.07.121. (2020).
6. **Zhang, F.**; Huang, C.; Xie, B.; Wu, X., Revisiting the chemical kinetics of CH3 + O-2 and its impact on methane ignition. *Combustion and Flame 200*, 125-134, (2019).
7. **Zhang, F.**; Huang, C., Pressure-Dependent Kinetics of the Reaction between CH3OO and OH Focusing on the Product Yield of Methyltrioxide (CH3OOOH). *Journal of Physical Chemistry Letters 10* (13), 3598-3603, (2019).
8. Huang, C.; Yang, B.; **Zhang, F.**, Calculation of the absolute photoionization cross-sections for C1-C4 Criegee intermediates and vinyl hydroperoxides. *Journal of Chemical Physics 150* (16), (2019).
9. Huang, C.; Yang, B.; **Zhang, F.**; Tian, G., Quantification of the resonance stabilized C4H5

isomers and their reaction with acetylene. *Combustion and Flame 198*, 334-341, (2018).

10. Zhang, P.; Li, S.; Wang, Y.; Ji, W.; Sun, W.; Yang, B.; He, X.; Wang, Z.; Law, C. K.; **Zhang, F.**, Measurement of reaction rate constants using RCM: A case study of decomposition of dimethyl carbonate to dimethyl ether. *Combustion and Flame 183*, 30-38, (2017).
11. Xing, L.; Zhang, L.; **Zhang, F.**; Jiang, J., Theoretical kinetic studies for low temperature oxidation of two typical methylcyclohexyl radicals. *Combustion and Flame 182*, 216-224, (2017).
12. Xing, L.; Bao, J. L.; Wang, Z.; **Zhang, F.**; Truhlar, D. G., Degradation of Carbonyl Hydroperoxides in the Atmosphere and in Combustion. *Journal of the American Chemical Society 139* (44), 15821-15835, (2017).
13. Huang, C.; Yang, B.; **Zhang, F.**, Pressure-dependent kinetics on the C4H7 potential energy surface and its effect on combustion model predictions. *Combustion and Flame 181*, 100-109, (2017).
14. Huang, C.; Yang, B.; **Zhang, F.**, Initiation mechanism of 1,3-butadiene combustion and its effect on soot precursors. *Combustion and Flame 184*, 167-175, (2017).
15. Xing, L.-L.; **Zhang, F.*;** Zhang L. -D., Theoretical studies for reaction kinetics of cy-C6H11CH2 radical with O2, *Proc. Combust. Inst.*, http://dx.doi.org/10.1016/j.proci.2016.08.050, 2016.
16. **Zhang, F.***; Nicolle, A.; Xing L. –L.; Klippenstein, S.J., Recombination of aromatic radicals with molecular oxygen, *Proc. Combust. Inst.*, http://dx.doi.org/10.1016/j.proci.2016.06.021, 2016.
17. Bian, H.-T.; Wang, Z.-D.; Sun, J.-H.; **Zhang, F.***, Conformational inversion-topomerization mechanism of ethylcyclohexyl isomers and its role in combustion kinetics, *Proc. Combust. Inst.*, http://dx.doi.org/10.1016/j.proci.2016.07.049, 2016.
18. Sun, W.-Y; Yang, B.;* Hansen, N.; Westbrook, C., **Zhang, F.**; Wang, G.; Moshammer, K.; Law. C. K., An Experimental and Kinetic Modeling Study on Dimethyl Carbonate (DMC) Pyrolysis and Combustion, *Combust. Flame* 164, 224-238 (2016)
19. Zhao, L.; Cheng, Z.-J; Ye, L.-L; **Zhang, F.**; Zhang, L.-D., Qi, F.; Li. Y.-Y., Experimental and kinetic modeling study of premixed o-xylene flames, *Proc. Combust. Inst.*, 35, 1745-1752 (2015).
20. Xing, L.-L.; Li, S.; Wang, Z-H.; Yang, B.; Klippenstein, S. J.; **Zhang, F.**,* Temperature and Pressure Dependent Uncertainty Analysis on RRKM/Master Equation Rate Constants: a Case Study for Ethanol Decomposition, Combust. Flame 162, 33427-3436 (2015).
21. Wang, Z. –D; Bian, H.-T; Wang, Y.; Zhang L.-D.;* Li, Y.-Y.; **Zhang F.***; Qi, F., Investigation on Primary Decomposition of Ethylcyclohexane at Atmospheric Pressure, *Proc. Combust. Inst.* 35, 367-375 (2015)
22. Wang, Z.-D; Zhao, L.; Wang, Y.; Bian, H.-T.; Zhang, L.-D.; **Zhang, F**.; Li, Y.-Y.; Sarathy, S. M.; Qi F.,* Kinetics of Ethylcyclohexane Pyrolysis and Oxidation: An Experimental and Detailed Kinetic Modeling Study, *Combust. Flame* 162, 2873-2892 (2015).
23. Jiao, Y.-G.; **Zhang, F**.; Dibble T.S.;* A Quantum Chemical Study of Autoignition of Methyl Butanoate, *J. Phys. Chem. A*, 119, 7282-7292 (2015)
24. Bian, H.-T.; Wang, Z.-H., **Zhang, F.;*** Wang, Z.-D., Unimolecular Reaction Properties

for the Long Chain Alkenyl Radicals, *Int. J. Chem. Kinet.* 47, 685-694 (2015).

25. Cheng, Z.-J.;, Xing, L.-L.; Zeng, M.-R.; **Zhang, F.**; Zhang, L.-D.; Qi, F.; Li, Y.-Y.; Experimental and Kinetic Modeling Study of 2,5-Dimethylfuran Pyrolysis at Various Pressures, *Combust. Flame* 161, 2496-2511 (2014)
26. Cai, J.-H.; Yuan, W.-H.; Ye, L.-L.; Cheng, Z.-J.; Wang, Y.-Z.; Dong, W.-L.; Zhang, L.-D.; Li, Y.-Y.; **Zhang, F.**;* Qi. F.;,* Experimental and Kinetic Modeling Study of i-butanol Pyrolysis and Combustion, *Combust. Flame* 161, 1955-1971 (2014).
27. Wang, Z.-D.; Ye, L.-L.; Yuan, W.-H.; Zhang, L.-D.; Wang, Y.-Z.; Cheng, Z.-J.; **Zhang**, **F**.;* Qi, F.;* Experimental and Kinetic Modeling Study on Methylcyclohexane Pyrolysis and Combustion, *Combust. Flame* 161, 84-100 (2014).
28. Wang, Z.-H.; Zhang, Z.-D.; **Zhang**, **F**.;* Kinetics of Homoallylic/Homobenzylic Rearrangement Reactions under Combustion Conditions, *J. Phys. Chem. A*, 118, 6741-6748 (2014).
29. Wang, Z.-D.; Li, Y.-Y.; **Zhang, F**.; Zhang, L.-D.; Yuan, W.-H.; Wang, Y.-Z.; Qi, F.;* An Experimental and Kinetic Modeling Investigation on a Rich Premixed n-propylbenzene Flame at Low Pressure, *Proc. Combust. Inst.* 34, 1785-1793 (2013).
30. Zhang, K.-W.; Zhang, L.-D.; Xie, M-F.; Ye, L.-L.; **Zhang, F.**; Glarborg, P.;*, Qi, F.,* An Experimental and Kinetic Modeling Study of Premixed Nitroethane Flames at Low Pressure, *Proc. Combust. Inst.* 34, 617-624 (2013).
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33. Jia, L.-Y.; Yang, J.-Z.; Zhang, L.-D.; **Zhang**, **F.**;* Qi, F.;* Fan, H.-Y.; Cai, J.-B., Experimental and Theoretical Studies of Pyrolysis of Chrysophanol and its Derivatives, *J. Anal. Appl. Pyro.* 100, 237-244 (2013).
34. **Zhang, F.**;* Wang, Z.-D.; Wang, Z.-H.; Zhang, L.-D.; Li, Y.-Y.; Qi, F., Kinetics of Decomposition and Isomerization of Methylcyclohexane: Starting Point for Studying Monoalkylated Cyclohexanes Combustion, *Energy Fuels* 27, 1679-1687 (2013).
35. Wang, Z.-D.; Cheng, Z.-J.; Yuan, W.-H.; Cai, J.-H.; Zhang, L.-D.; **Zhang, F.**; Qi, F.,* Wang, J., An Experimental and Kinetic Modeling Study of Cyclohexane Pyrolysis at Low Pressure, *Combust. Flame* 159, 2243-2253 (2012).
36. Dibble, T. S.;* Sha, Y.; Thornton, W. F.; **Zhang, F.**, Cis-Trans Isomerization of Chemically Activated 1-Methylallyl Radical and Fate of the Resulting 2-Buten-1-peroxy Radical, *J. Phys. Chem. A* 116, 7603-7614 (2012).
37. Cai, J.-H.; Zhang, L.-D.; **Zhang, F.**; Wang, Z.-D.; Cheng, Z.-J.; Yuan, W.-H.; Qi, F.,* A Comprehensive Experimental and Kinetic Modeling Study of *n*-butanol Pyrolysis and Combustion, *Energy Fuels* 26, 5550-5568 (2012).
38. Yang, J.-Z.; **Zhang, F.**; Jia, L.-Y.; Zhang, L.-D.;* Qi, F.; Fan, H.-Y.; Cai, J.-B., Experimental and Theoretical Study on Pyrolysis of Isopsoralen, *Chin. J. Chem. Phys*. 25, 249-253 (2012).
39. Ye, L.-L.; **Zhang, F.**; Zhang, L.-D.;*, Qi F., Theoretical Studies on the Unimolecular

Decomposition of Propanediols and Glycerol, *J. Phys. Chem. A* 116, 4457-4465 (2012).

40. Zhao, L.; Ye, L.-L.; **Zhang, F.**;* Zhang, L.-D.,* Thermal Decompostion of 1-pentanol and its Isomers: a Theoretical study, *J. Phys. Chem. A* 116, 9238-9244 (2012).
41. **Zhang, F.**; Dibble, T. S.;* Effects of olefin functional group and its position on kinetics of unimolecular reactions of peroxy radicals, *J. Phys. Chem. A* 115, 655-663 (2011).
42. **Zhang, F.;** Dibble, T. S.;* Impact of Tunneling Effect on Hydrogen-migration of n-propyl Peroxy Radical, *Phys. Chem. Chem. Phys*. 13, 17969-17977 (2011). (cover article)
43. Ai, Y.-J.; **Zhang, F.**; Fang, W.-H.;* Luo, Y.;* Importance of the Intra-hydrogen Bonding on the Photochemistry of Anionic Hydroquinone (FADH-) in DNA Photolyase, *J. Phys. Chem. Lett.* 1, 743-747 (2010).
44. Cui, G.-L.; **Zhang, F**.; Fang, W.-H.;* Insights into the Mechanistic Photodissociation of Methyl Formate, *J. Chem. Phys.* 132, 034306 (2010).
45. **Zhang, F.**; Ai, Y.-J.; Luo, Y.;* Fang, W.-H.,* Nonadiabatic Histidine Dissociation of Hexacoordinate Heme in Neuroglobin Protein, *J. Phys. Chem. A*. 114,1980-1984 (2010).
46. Ai, Y.-J.; **Zhang, F.**; Fang, W.-H.;*, Luo, Y.,* Ultrafast Deactivation Processes in the 2-Aminopyridine Dimer and the A-T Base Pair: Similarities and Differences, *J. Chem. Phys*. 133, 064302 (2010).
47. **Zhang, F.**; Fang, W.-H.;* Luo, Y.,* A multi-dimensional microcanonical Monte Carlo study of S-0 -> T-1 intersystem crossing of isocyanic acid, *Sci. China, Ser. B-Chem.*, 52, 1885-1891 (2009).
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50. Cui, G.-L.; Li, Q.-S.; **Zhang, F**.; Fang, W.-H.;* Yu, J.-G.,* Combined CASSCF and MR-CI Study on Photoinduced Dissociation and Isomerization of Acryloyl Cholorid, *J. Phys. Chem. A* 110, 11839-11846 (2006).
51. Zhang, F.; Ding, W.-J.; Fang, W.-H., Combined nonadiabatic transition-state theory and ab initio molecular dynamics study on selectivity of the alpha and beta bond fissions in photodissociation of bromoacetyl chloride, *J. Chem. Phys.* 125, 184305 (2006).
52. Li, Q.-S.; **Zhang, F.**; Fang, W.-H.;* Yu,J.-G., Probing Mechanistic Photochemistry of Glyoxal in the Gas Phase by ab initio Calculations of Potential-energy Surfaces and Adiabatic and Nonadiabatic Rates, *J. Chem. Phys.*124, 054324 (2006).
53. Fang, W.-H.;* **Zhang, F**.; Li, Q.-S.; Chen, S.-L., Probing Mechanistic Photodissociation of Carbonyl Compounds from ab Initio Calculations, Molecular Dynamics Simulations, and non-Adiabatic Rates, *Trends in Chemical Physics* 13, 1-27 (2006).
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55. Lin, L.; **Zhang, F.**; Fang, W.-H.,* Striving to Understand the Photophysics and Photochemistry of Thiophosgene: A Combined CASSCF and MR-CI Study, *J. Phys.*

Chem. A 109, 554-561 (2005).

56. **Zhang, F**.; Lin, L.; Fang, W.-H.,* Insights into Dynamics of the S2 State of Thiophosgene from ab Initio Calculations, *J. Chem. Phys.* 121, 6830-6834 (2004).