

Dequan Xiao, Ph. D.

Associate Professor & Endowed Jacob F. Buckman Chair
Director, Center for Integrative Materials Discovery
Coordinator, Graduate Program in Chemistry

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EDUCATION

- **Postdoc, Yale University**, Theoretical and Computational Chemistry, 2009-2013
- **PhD, Duke University**, Theoretical and Computational Chemistry, 2009
- **MS, University of Central Florida**, Industrial Chemistry, 2003
- **MS, Sichuan University (China)**, Polymer Chemistry, 1999
- **BS, Sichuan University (China)**, Chemistry, 1996

EMPLOYMENT HISTORY

University of New Haven, Department of Chemistry and Chemical Engineering

Assistant Professor: August 2013 – August 2019

Associate Professor: September 2019 --

Yale University, Department of Chemistry

Postdoctoral Research Associate: August 2009 – April 2012

Associate Research Scientist: May 2012 – July 2013

Duke University, Department of Chemistry

Visiting Scholar: May 2009 – July 2009

Graduate Research Assistant: August 2003 – May 2009

University of Central Florida, Department of Chemistry

Graduate Research Assistant: August 2001 - July 2003

Sichuan University (China), Department of Chemistry

Lecturer: July 1999 – August 2001

Graduate Research Assistant: September 1996 - July 1999

AWARDS AND HONORS

- Buckman Chair Endow Professor, 2019-2022, University of New Haven
- University Research Scholar, 2016-2019, University of New Haven
- Conference Travel Grant, 2008, Duke University
- University Merit Fellowship, 2002, University of Central Florida
- Procter & Gamble Outstanding Graduate Student Fellowship, 1998, Sichuan University
- Admitted into the M.S. chemistry program the exemption of standardized national entrance exams due to the academic excellence, 1996, Sichuan University
- Annual Academic Excellence Fellowships, 1993-1996, Sichuan University
- Excellence Prize in Chemistry Olympic Match for High School Students, 1991, Guangdong Province

GRANT AWARDS

16. PI, Buckman Chair Endow Professorship Award, University of New Haven, \$90,000 07/2019-06/2022
15. PI, Summer Research Grant and Research Fund, University of New Haven, \$3,250, 07/2019-06/2019
14. PI, Industrial contract grant, Higasket Plastics Group Co. Ltd, \$332,576, 08/2018-07/2020
Title: "Optimizing Polymer Complex Materials by Integrative Approaches"
13. Senior Personnel, NSF-MRI award (PI, Dr. Brooke W. Kammarath), \$317,357, 09/2018-02/2020
"MRI: Acquisition of Laser Induced Breakdown Spectrometers (LIBS)"
12. PI, Industrial contract grant, Higasket Plastics Group Co. Ltd, \$221,429, 07/2017-07/2018
Title: "Integrative Analysis of Polymer Complex Materials"
11. PI, University Research Scholar Research Fund, University of New Haven, \$12,000, 05/2016-04/2019
Title: "Inverse Molecular Design of Green Catalysts for Biomass Conversion"
10. PI, Summer Research Grant and Research Fund, University of New Haven, \$5,250, 07/2016-06/2017
9. PI, Research fund from Higasket Plastics Group Co. Ltd., \$100,000, 06/2016-05/2021
Title: "Founding the Higasket Polymer Materials Laboratory"
8. Co-PI, a team proposal awarded by Connecticut Biolnovative Program through the Program in Innovative Therapeutics for Connecticut Health (PITCH) at Yale University with PI, Dr. Jun Lu (Yale University), 2015-2016.
Title: "Discover Small Molecule Modulators of Tumor Suppressors for Leukemia Disease"
7. Senior Personnel, NIH award (PI, Dr. Narendra Wayajapee at Yale University), \$278,877, 3/2016-2/2017

Title: "Small molecule inhibitors targeting oncogenic drivers of hepatocellular carcinoma".

6. PI, Summer Research Grant and Research Fund, University of New Haven, \$4,750, 07/15-06/16

5. Senior Personnel, NSF-MRI award (PI, Dr. Nancy Savage), \$197,376, 09/2015-02/2017
"MRI: Acquisition of an X-Ray Diffraction (XRD) System"

4. PI, Summer Research Grant and Research Fund, University of New Haven, \$5,250, 07/2014-06/2015

3. PI, Sub-contract for an NSF award to Yale University, \$5,816, 07/2014-01/2015
Sub-contract Title: "Computational study of photoabsorption properties and bond dissociation energies for a library of toxic organic molecules"

Original NSF award (PI, Dr. Paul Anastas at Yale University): \$4,598,705, 9/13-8/17

Title: "NSMDS: Improving Material Safety through the Minimization of Oxidative Stress Potential: A mechanistic understanding of ROS generation in in vitro and in vivo systems"

2. PI, Industry contract from L2 Diagnostics LLC, \$6,000, 09/2014-09/2015

1. PI, Collaboration fund with Yale University, \$720, 08/2013-11/2013

Title: "Computational study of molecular dynamics and catalytic mechanism for TET2 proteins"

PROFESSIONAL MEMBERSHIPS

- Member, American Chemical Society.
- Member, American Physical Society.
- Member, Sigma Xi, the Scientific Research Society.

COURSE TEACHING

University of New Haven

- Physical Chemistry I and II
- Physical Chemistry Laboratory
- Introduction to Computational Chemistry
- Polymer Science/Biomedical Polymers

Duke University

- Organic Chemistry Laboratory
- Computational Chemistry
- General Chemistry Laboratory

University of Central Florida

- Organic Chemistry Laboratory
- General Chemistry Laboratory

Sichuan University

- Polymer Materials Science and Engineering

- Polymer Chemistry and Physics Laboratory

ACADEMIC SERVICES

- **Journal Reviewer:**
Journal of American Chemical Society, Green Chemistry, Journal of Physical Chemistry Letters, Journal of Chemical Theory and Computation, Journal of Physical Chemistry, ACS Applied Materials and Interfaces, ACS Omega, Nature-Scientific Data, Nature Communications, Journal of Materials Chemistry, RSC Advances, RSC Open Science, Diamond and Related Materials, Journal of Applied Polymer Science, Journal of Molecular Modeling, MPDI-Molecules, MPDI-Catalysts, MPDI-Algorithms, Journal of Mathematical Bioscience, Computational and Theoretical Chemistry, the Korean Journal of Chemical Engineering, Sensors & Actuators: B. Chemical, Computing in Science and Engineering, Solid-State Ionics, Journal of Inorganic Biochemistry, Applied Science, Journal of Environmental Chemical Engineering, Journal of Polymer Research
- **Grant Reviewer:**
National Science Foundation Panelist, NASA CT Space Grant Consortium, National Science Centre (Poland)
- **Advisory Board:**
NASA Connecticut Space Grant Consortium
- **Educational Programs:**
One of the founding faculty of a new Biomedical Engineering MS program at the University of New Haven in 2014
Original developer for a new chemistry-MS program (with a uniquely designed *integrative approach* curriculum for chemistry graduate education) at the University of New Haven in 2017 (and new program was approved by the university and the State.)

PUBLICATIONS

According to Google Scholar in December, 2018, total number of citations: 1061, h-index: 18

- **PhD dissertation**
Dequan Xiao, "Molecular Design for Nonlinear Optical Materials and Molecular Interferometers Using Quantum Chemistry Calculations", Duke University, **2008**.

Research Articles or Reviews

2020

64. Huizhu Cai, Bingbing Chen, Xiao Zhang, Yuchen Deng, **Dequan Xiao**, Ding Ma, and Chuan Shi, "Highly Active Sites of Low Spin Fe^{II}N₄ Species: the Identification and the ORR Performance", *Manuscript*, **2020**, submitted.

63. Jiliang Ma, Dongnv Jin, Yancong Li, **Dequan Xiao**, Gaojie Jiao, Yanzhu Guo, Lingping Xiao, Xiaohong Chen, Xinze Li, Jinghui Zhou, and Runcang Sun, "Photocatalytic Conversion of Biomass-

Based Monosaccharides to Lactic Acid by Ultrathin Porous Oxygen Doped Carbon Nitride”, *Manuscript*, **2020**, submitted.

62. Hanxi Bao, William J. Sagues, Yigui Wang, Shunchang Yang, **Dequan Xiao**, and Zhaohui Tong, “Catalytic Depolymerization of Lignin to Monophenolic Compounds Using Low-Cost Biomimetic Persulfate Catalyst Under Mild Conditions”, *Manuscript*, **2020**, to be submitted.

61. Michael Orsini, Johnny Chang, Laurene Petitjean, David Landofi, William Schwartz, Lin Zhang, Zhaohui Tong, Paul T. Anastas, and **Dequan Xiao**, “Design Heterogeneous Catalysts for Lignin Degradation Guided by Inverse Molecular Design Theory”, *Manuscript*, **2020**, to be submitted.

60. Pashupati Pokharel, Feng Wei, and **Dequan Xiao**, “Thermomechanical Properties of Polypropylene and Styrene-ethylene-butylene-styrene Blends: A Molecular Simulation and Experimental Study”, *Manuscript*, **2020**, to be submitted.

59. Danielle S. Hanson, Yigui Wang, Xinrui Zhou, Erik Washburn, Merve B. Ekmekci, Donovan Dennis, Amay Paripati, **Dequan Xiao**, Meng Zhou “An Experimental and Computational Study of the Catalytic Formation of Urea from Ammonium Carbamate using a Copper(II) Complex”, *Manuscript*, **2020**, to be submitted.

58. Chunyang Dong, Yinlong Li, Danyang Cheng, Mengtao Zhang, Jinjia Liu, Yang-Gang Wang, Dequan Xiao, and Ding Ma “Supported Metal Clusters Catalysts: Roles of Their Unique Geometric and Electronic Structures in Heterogeneous Catalysis”, *Manuscript*, **2020**, submitted.

57. Chuqiao Song, Xi Liu, Ming Xu, Daniel Masi, Yigui Wang, Yuchen Deng, Mengtao Zhang, Xuetao Qin, Kai Feng, Jie Yan, Jing Leng, Zhaohua Wang, Yao Xu, Binhang Yan, Shengye Jin, Dongsheng Xu, Zhen Yin, **Dequan Xiao**, Ding Ma “Photothermal Conversion of CO₂ with Tunable Selectivity using Iron-Based Catalysts”, *Manuscript*, **2020**, Submitted.

56. Jijiao Zeng, Zhaohui Tong, Hanxi Bao, Nusheng Chen, Fei Wang, Yigui Wang, **Dequan Xiao**, “Controllable Degradation of Lignin Using Carbocatalyst Graphene Oxide Under Mild Conditions” *Fuel*, **267**, **2020**, 1171000. (IF=5.1)

2019

55. Xiaohui He, Yuchen Deng, Ying Zhang, Qian He, **Dequan Xiao**, Mi Peng, Yue Zhao, Hao Zhang, Rongchang Luo, Tao Gan, Hongbing Ji, and Ding Ma, “Mechanochemical Kilogram-Scale Synthesis of Noble Metal Single-Atom Catalysts” *Cell Reports Physical Science*, **1**, **2019**, 100004.

54. Trevor Callahan, Daniel Masi, and **Dequan Xiao**, “Designing Catalytic Sites on Surfaces with Optimal H-Atom Binding via Atom Doping Using the Inverse Molecular Design Approach” *Journal of Physical Chemistry B*, **123**(48), **2019**, 10252-10259. (IF=2.9)

53. Jia-Jia Yang, Xiang-Yang Liu, Wei-Hai Fang, **Dequan Xiao**, and Ganglong Cui, “Photoinduced Carrier Dynamics at the Interface of Black Phosphorus and Bismuth Vanadate” *Journal of Physical Chemistry A*, **123**(46), **2019**, 10019-10029. (IF=2.8)

52. Fei Huang, Yuchen Deng, Yunlei Chen, Xiangbin Cai, Mi Peng, Zhimin Jia, Jinglin Xie, **Dequan Xiao**, Xiaodong Wen, Ning Wang, Zheng Jiang, Hongyang Liu, and Ding Ma “Anchoring Cu₁ species over nanodiamond-graphene for semi-hydrogenation of acetylene” *Nature Communications*, **10**, **2019**, 4431. (IF=12.4)

51. Yuchen Deng, Yuzhen Ge, Ming Xu, Qiaolin Yu, **Dequan Xiao**, Siyu Yao, and Ding Ma “Molybdenum carbide: controlling the geometric and electronic structure of noble metals for the activation of O-H and C-H bonds” *Accounts of Chemical Research*, **2019**, **52**(12), 3372-3383. (IF=21.7)

50. Renxi Jin, Mi Peng, Ang Li, Yuchen Deng, Zhimin Jia, Fei Huang, Yunjian Ling, Fan Yang, Xiaodong Han, **Dequan Xiao**, Zheng Jiang, Hongyang Liu, and Ding Ma, "Low Temperature Oxidation of Ethane to Oxygenates by Oxygen over Iridium-Cluster Catalysts" *Journal of American Chemical Society*, 141(48), 2019, 18921-18925. (IF=14.4)

49. Siwei Li, Jinghe Yang, Chuqiao Song, Qingjun Zhu, **Dequan Xiao**, Ding Ma "Iron Carbides: Control Synthesis and Catalytic Applications in CO_x Hydrogenation and Electrochemical HER" *Advanced Materials*, 2019, 1901796. (IF=25.8)

48. Xiaohui He, Qian He, Yuchen Deng, Mi Peng, Hongyu Chen, Ying Zhang, Siyu Yao, Mengtao Zhang, **Dequan Xiao**, Ding Ma, Binghui Ge, and Hongbing Ji "A versatile route to fabricate single atom catalysts with high chemoselectivity and regioselectivity in hydrogenation" *Nature Communications*, 10, 2019, 3663. (IF=12.4)

47. Pengqi Yan, Wenhan Guo, Zibin Liang, Wei Meng, Zhen Yin, Siwei Li, Mengzhu Li, Mengtao Zhang, Jie Yan, **Dequan Xiao**, Ruqiang Zou, Ding Ma "Highly efficient K-Fe/C catalysts derived from metal-organic frameworks towards ammonia synthesis" *Nano Research*, 2019, 1-7. (IF=8.0)

46. Jiayun Zhang, Yuchen Deng, Xiangbin Cai, Yunlei Chen, Mi Peng, Zhimin Jia, Zheng Jiang, Pengju Ren, Siyu Yao, Jinglin Xie, **Dequan Xiao**, Xiaodong Wen, Ning Wang, Hongyang Liu, and Ding Ma "Tin Assisted Fully Exposed Platinum Clusters Stabilized on Defect-Rich Graphene for Dehydrogenation Reaction" *ACS Catalysis*, 9(7), 2019, 5998-6005. (IF=11.4)

45. Yao Xu, Jing Li, Wenjing Li, Weizhen Li, Xiaochen Zhang, Yue Zhao, Jinglin Xie, Xiaoping Wang, Xi Liu, Yongwang Li, **Dequan Xiao**, Zhen Yin, Yong Cao, and Ding Ma "Direct conversion of CO and H₂O into liquid fuels under mild conditions" *Nature Communications*, 10, 2019, 1389. (IF=12.4)

44. Zhaoxuan Wu, Bing Yang, Shu Miao, Wei Liu, Jinglin Xie, Sungsik Lee, Michael J Pellin, Dequan Xiao, Dangsheng Su, and Ding Ma, "Lattice strained Ni-Co alloy as high-performance catalyst for catalytic dry-reforming of methane" *ACS Catalysis*, 9, 2019, 2693-2700. (IF=11.4)

43. Pashupati Pokharel, **Dequan Xiao**, Folarin Erogbogbo, Ozgur Keles, "A novel approach for creating conductive network structure in polyurethane nanocomposites using a hybrid of graphene nanoplatelets, carbon black and multi-walled carbon nanotubes", *Composites Part B: Engineering*, 161, 2019, 169-182. (IF=4.9)

2018

42. Jiliang Ma, Zewei Liu, Junlong Song, Linxin Zhong, **Dequan Xiao**, Hongxia Xi, Xuehui Li, Run-Cang Sun and Xinwen Peng, "Au@h-Al₂O₃ analogic yolk-shell nanocatalyst for highly selectively synthesis of biomass-derived D-xylonic acid via regulation of structure effect" *Green Chemistry*, 20, 2018, 5188-5195. (IF=8.6)

41. Siyu Yao, **Dequan Xiao**, Ding Ma, "Observing How Fischer-Tropsch Synthesis Catalysts Work at the Nanoscale in Real Time Using Operando Scanning Transmission X-ray Microscopy" (Preview) *Chem (Cell Press)*, 4, 2018, 2493-2495. (IF=14.1)

40. Fei Huang, Yuchen Deng, Yunlei Chen, Xiangbin Cai, Mi Peng, Zhimin Jia, Pengju Ren, **Dequan Xiao**, Xiaodong Wen, Ning Wang, Hongyang Liu, and Ding Ma, "Atomically Dispersed Pd on Nanodiamond/Graphene Hybrid for Selective Hydrogenation of Acetylene" *Journal of American Chemical Society*, 140(41), 2018, 13142-13146. (IF=14.4)

39. Yang Li, Liyuan Kuang, **Dequan Xiao**, Appala Raju Badireddy, Maocong Hu, Shiqiang Zhuang, Xianqin Wang, Eon Soo Lee, Taha Marhaba, and Wen Zhang, "Hydrogen Production from Organic

Fatty Acids using Carbon-Doped TiO₂ Nanoparticles under Visible Light Irradiation" *International Journal of Hydrogen Energy*, 43(9), 2018, 4335-4346. (IF=4.2)

38. Yueshen Wu, Benjamin Rudshiteyn, Ingolf Warnke, **Dequan Xiao**, Victor S. Batista, "Mechanistic study of CO/CO₂ conversion catalyzed by a biomimetic Ni(II)-iminothiolate complex", *International Journal of Quantum Chemistry*, 118, 2018, e25555. (IF=2.6)

2017

37. **Dequan Xiao** and Trevor Callahan, "The role of atomic orbitals of doped earth-abundant metals on designed copper catalytic surfaces", 2017, arXiv:1701.04333.

36. Laurene Petitjean, Raphael Gagne, Evan S. Beach, Jason An, Paul T. Anastas, and Dequan Xiao, "Quantum Chemistry Analysis of Reaction Thermodynamics for Hydrogenation and Hydrogenolysis of Aromatic Biomass Model Compounds", *ACS Sustainable Chemistry and Engineering*, 5(11), 2017, 10371-10378. (IF=6.1)

35. **Dequan Xiao**, Rui Hu, "A Tutorial of the Inverse Molecular Design Theory in Tight-Binding Frameworks and Its Applications", Chapter 8, in "Handbook of Green Chemistry V10 – Tools for Green Chemistry", Ed. Paul T. Anastas, Evan S. Beach, Soumen Kundu, 2017, Wiley Publishers.

2016

34. Laurene Petitjean, Raphael Gagne, Evan S. Beach, **Dequan Xiao**, and Paul T. Anastas, "Highly Selective Hydrogenation and Hydrogenolysis using a Copper doped Porous Metal Oxide Catalyst", *Green Chemistry*, 18(1), 2016, 150-156. (IF=8.6)

33. Weixin Huang, Shiran Zhang, Y. Tang, Yuanyuan Li, Luan Nguyen, Junjun Shan, **Dequan Xiao**, Raphael Gagne, Anatoly I. Frenkel, Franklin (Feng) Tao, "Low-Temperature Transformation of Methane to Methanol on Single Sites Anchored on Internal Surface of Microporous Silicate in Liquid", *Angewandte Chemie International Edition*, 43, 2016, 13639-13643. (IF=12.0)

32. Aimin Ge, Benjamin Rudshiteyn, Brian T. Psciuk, **Dequan Xiao**, Jia Song, Chantelle L. Anfusio, Allen M. Ricks, Victor S. Batista, and Tianquan Lian, "Surface-Induced Anisotropic Binding of a Rhenium CO₂-Reduction Catalyst on Rutile TiO₂(110) Surfaces", *Journal of Physical Chemistry C*, 120(37), 2016, 20970-20977. (IF=4.5)

2015

31. Jun Yuan, Yingping Zou, Ruili Cui, Yi-Hsiang Chao, Zaiyu Wang, Mingchao Ma, Yuehui He, Yongfang Li, Amanda Rindgen, Wei Ma, **Dequan Xiao**, Zhishan Bo, Xinjun Xu, Lidong Li, and Chain-Shu Hsu, "Incorporation of Fluorine onto Different Positions of Phenyl Substituted Benzo[1,2-b:4,5-b']dithiophene Unit: Influence on Photovoltaic Properties", *Macromolecules*, 48(13), 2015, 4347-4356. (IF=5.9)

30. Li Fu, Zhuguang Wang, Brian T. Psciuk, **Dequan Xiao**, Victor S. Batista, Elsa C. Y. Yan, Characterization of Parallel β -sheets at Interfaces by Chiral Sum Frequency Generation Spectroscopy, *Journal of Physical Chemistry Letters*, 6, 2015, 1310-1315. (IF=8.7)

29. **Dequan Xiao** and Evan S. Beach, "Green Catalysts for Producing Liquid Fuels from Lignocellulosic Biomass", in: *Worldwide Trends in Green Chemistry Education*, eds V. Zuin and L. Mammino, Royal Society of Chemistry, Cambridge, 978-1-84973-949-8, 2015.

28. Brian T. Psciuk, Mirabelle Premont-Schwarz, Benjamin Koeppel, Sharon Keinan, **Dequan Xiao**, Erik T. J. Nibbering, and Victor S. Batista, "The O-H Stretching Mode of Aromatic Alcohols as an Ultrafast Local Probe of Photoacidity in Hydrogen-Bonded Complexes", *Journal of Physical Chemistry A*, **119**(20), **2015**, 4800-4812. (IF=2.8)

2014

27. Cheng Jin, Taoran Zhang, Lingyu Wang, Meiyong He, Tinglian Yuan, Bo Jiang, **Dequan Xiao** and Qinjian Yin, "Photoinduced Deformation of Hollow Nanospheres Formed by the Self-Assembly of Amphiphilic Random Copolymers and Small Azo Molecules", *RSC Advances*, **4**, **2014**, 45890-45894. (IF=2.9)

26. Cheng Jin, Taoran Zhang, Fangzhuang Liu, Lingyu Wang, Qinjian Yin, and **Dequan Xiao**, "Fabrication of Size Controllable Polymeric Hollow Nanospheres Containing Azo Functional Groups via Ionic Self-Assembly", *RSC Advances*, **4**, **2014**, 8216-8223. (IF=2.9)

25. Omar F. Mohammed, **Dequan Xiao**, Victor S. Batista, and Erik T. J. Nibbering, "Excited-State Intramolecular Hydrogen Transfer (ESIHT) of 1,8-Dihydroxy-9,10-anthraquinone (DHAQ) Characterized by Ultrafast Electronic and Vibrational Spectroscopy and Computational Modeling", *Journal of Physical Chemistry A*, **118**(17), **2014**, 8216-8223. (IF=2.8)

24. **Dequan Xiao**, Ingolf Warnke, Jason Bedford, and Victor S. Batista, "Inverse Molecular Design for Materials Discovery", *RSC Specialist Periodical Report -- Chemical Modelling*, **10**, **2014**, 1-31.

2013

23. Li Fu, **Dequan Xiao**, Zhuguang Wang, Victor S. Batista, and Elsa C. Yan, "Chiral Sum Frequency Generation for In Situ Probing Proton Exchange in Antiparallel Beta-Sheets at Interfaces", *Journal of American Chemical Society*, **135**, **2013**, 3592-3598. (IF=14.4)

22. Chetan Poojari, **Dequan Xiao**, Birgit Strodel, and Victor S. Batista, "Membrane Permeation Induced by Aggregates of Human Islet Amyloid Polypeptides", *Biophysical Journal*, **105**, **2013**, 2323-2332. (IF=3.5)

21. Fabrizio Messina, Mirabelle Prémont-Schwarz, Olivier Braem, **Dequan Xiao**, Victor S. Batista, Erik T. J. Nibbering, and Majed Chergui, "Ultrafast Solvent-Assisted Electronic Level Crossing in 1-Naphthol", *Angewandte Chemie International Edition*, **52**(27), **2013**, 6871-6875. (IF=12.0)

2012

20. Xuwen Chen, Bo Liu, Yingping Zou, Wangjun Tang, Yongfang Li, and **Dequan Xiao**, "Copolymers from Naphtho[2,3-c]thiophene-4,9-dione Derivatives and Benzodithiophene: Synthesis and Photovoltaic Applications", *RSC Advances*, **2**(19), **2012**, 7439-7448. (IF=2.9)

19. Ping Ding, Yingping Zou, Chengche Chu, **Dequan Xiao**, and Chain-Shu Hsu, "Effects of Thiophene Units on Substituted Benzothiadiazole and Benzodithiophene Copolymers for Photovoltaic Applications", *Journal of Applied Polymer Science*, **125**(5), **2012**, 3936-3945. (IF=1.9)

18. Ping Ding, Cheng-Che Chu, Yingping Zou, **Dequan Xiao**, Chunyue Pan, and Chain-Shu Hsu "New Low Bandgap Conjugated Polymer Derived from 2, 7-Carbazole and 5, 6-Bis(octyloxy)-4, 7-Di(thiophen-2-yl) Benzothiadiazole: Synthesis and Photovoltaic Properties", *Journal of Applied Polymer Science*, **123**(1), **2012**, 99-107. (IF=1.9)

17. Dequan Xiao, Li Fu, Jian Liu, Victor S. Batista, and Elsa C. Yan, "Amphiphilic Adsorption of Human Islet Amyloid Polypeptide Aggregates to Lipid/Aqueous Interfaces", *Journal of Molecular Biology*, 421, 2012, 537-547. (IF=4.9)

16. Chantelle L. Anfuso, Dequan Xiao, Allen M. Ricks, Christian F. A. Negre, Victor S. Batista, and Tianquan Lian, "Orientation of a Series of CO₂ Reduction Catalysts on Single Crystal TiO₂ Using Phase-Sensitive Vibrational Sum Frequency Generation Spectroscopy (PS-VSFGS)", *Journal of Physical Chemistry C*, 116(45), 2012, 24107-24114. (IF=4.5)

2011

15. Chantelle Anfuso, Robert C. Snoeberger III, Allen Ricks, Weimin Liu, Dequan Xiao, Victor S. Batista, and Tianquan Lian, "Covalent Attachment of a Rhenium Bipyridyl CO₂ Reduction Catalyst to Rutile TiO₂", *Journal of American Chemical Society*, 133(18), 2011, 6922-6925. (IF=14.4)

14. Dequan Xiao, Lauren A. Martini, Robert C. Snoeberger III, Robert H. Crabtree, and Victor S. Batista, "Inverse Design and Synthesis of acac-Coumarin Anchors for Robust TiO₂ Sensitization", *Journal of American Chemical Society*, 133(23), 2011, 9014-9022. (IF=14.4)

13. Mirabelle Prémont-Schwarz, Dequan Xiao, Victor S. Batista, and Erik T. J. Nibbering, "The O-H Stretching Mode of a Prototypical Photoacid as a Local Dielectric Probe", *Journal of Physical Chemistry A*, 115(38), 2011, 10511-10516. (IF=2.8)

12. Dequan Xiao, Mirabelle Prémont-Schwarz, Erik T. J. Nibbering, and Victor S. Batista, "Ultrafast Vibrational Frequency Shifts Induced by Electronic Excitations: Naphthols in Low Dielectric Media", *Journal of Physical Chemistry A*, 116(11), 2011, 2775-2790. (IF=2.8)

2010

11. Kunhua Lin, Jing Sha, Yongchao Zhao, Ming Liu, Bo Jiang, Dequan Xiao, and Qinjian Yin, "Synthesis and Characterization of Azobenzene Chromophore Containing Polymeric Nanospheres", *Chemical Journal of Chinese University*, 31(10), 2010, 2067-2073. (IF=0.7)

10. Jing Sha, Kunhua Lin, Yongchao Zhao, Ming Liu, Bo Jiang, Dequan Xiao, and Qinjian Yin, "Study on the Aggregation Morphology of Side-Chain Azocomplex Synthesized by Ionic Self-Assembly", *Acta Chimica Sinica*, 68(20), 2010, 2111-2118. (IF=2.1)

9. Xiangqian Hu, Dequan Xiao, Shahar Keinan, Weitao Yang, Michael J. Therien, Koen Clays, and David N. Beratan, "Predicting the Frequency Dispersion of Electronic Hyperpolarizabilities on the Basis of Absorption Data and Thomas-Kuhn Sum Rules", *Journal of Physical Chemistry C*, 114(5), 2010, 2349-2359. (IF=4.5)

2009

8. Bo Liu, Hamed Najari, Chunxue Pan, Mario Leclerc, Dequan Xiao, and Yingping Zou, "New Low Bandgap Dithienylbenzothiadiazole Based Copolymers: Synthesis and Photovoltaic Properties", *Macromolecular Rapid Communications*, 31(4), 2009, 391-398. (IF=4.3)

7. David N. Beratan, Spiros S. Skourtis, Ilya A. Balabin, Alexander Balaeff, Shahar Keinan, Ravindra Venkatramani, and Dequan Xiao, "Steering Electrons on Moving Pathways", *Account of Chemical Research*, 40(10), 2009, 1669-1678. (IF=21.0)

6. **Dequan Xiao**, Spiros S. Skourtis, Igor V. Rubtsov, and David N. Beratan, "Turning Charge-Transfer On and Off in a Molecular Interferometer with Vibronic Pathways", *Nano Letters*, 9(5), **2009**, 1818-1823. (IF=12.1)

5. Zhiwei Lin, Candace M. Lawrence, **Dequan Xiao**, Victor V. Kireev, Spiros S. Skourtis, Jonathan L. Sessler, David N. Beratan, and Igor V. Rubtsov, "Modulating Unimolecular Charge Transfer by Exciting Bridge Vibrations", *Journal of American Chemical Society*, 131(50), **2009**, 18060-18062. (IF=14.4)

2008

4. **Dequan Xiao**, Felipe A. Bulat, Weitao Yang, and David N. Beratan, "A Donor-Nanotube Paradigm for Nonlinear Optical Materials", *Nano Letters*, 8(9), **2008**, 2814–2818. (IF=12.1)

3. **Dequan Xiao**, Weitao Yang, and David N. Beratan, "Inverse Molecular Design in a Tight-Binding Framework", *Journal of Chemical Physics*, 129(4), **2008**, 044106. (IF=2.8)

Prior to 2008

2. **Dequan Xiao**, Deben Chen, Zonghua Zhou, and Anyong Zhong, "Three-group Type Mechanism in the Curing Behavior of Polyacrylate and Blocked Toluene Diisocyanate", *Journal of Applied Polymer Science*, 83, **2002**, 112-120. (IF=1.9)

1. Anyong Zhong, Deben Chen, **Dequan Xiao**, and Zonghua Zhou, "Preparation and Curing Behavior of Blocked Isocyanate Crosslinkers", *Polymer Materials Science and Engineering (Chinese)*, 16, **2000**, 32-35.

- **Patents**

5. Polymeric Nanocompositions Comprising Self-Assembled Organic Quantum Dots, **US Patent App.** 12/208,307, 2008.

4. Qihai Xiao and **Dequan Xiao**, "Low-Smoke Halogen-Free Expansion Flame-Retarded Polyolefin Material for Electrical Plug and Its Preparing Method", **China Patent**, 200510101715.

3. Qihai Xiao and **Dequan Xiao**, "Low-Smoke Halogen-Free Expansion Flame-Retarded Polyolefin Electric-Wire External Material, Insulated Material and Its Preparing Method", **China Patent**, 200510101716.

2. Qihai Xiao and **Dequan Xiao**, "Low Smoke Non-Halogen Fire Retarding Expansive Polyolefins Electronic Wire Material and Preparation Process Thereof", **China Patent**, 200510121080.

1. Qihai Xiao and **Dequan Xiao**, "Smokeless and Halogen-Free Expanding Fire-Retardant Electric Wire Materials with Thermoplastic Elastomer and Production Thereof", **China Patent**, 200510121081.

- **Oral presentations**

39. **Dequan Xiao**, "Inverse Molecular Design of Green Catalysts for Converting Biomass into Value-Added Chemicals", Invited Seminar at Dalian Chemical Physics Institute (Dalian, China), June 28, **2019**.

- 38. Dequan Xiao**, "Inverse Molecular Design of Green Catalysts for Converting Biomass into Value-Added Chemicals", Invited Seminar at Huzhou University (Huzhou, China), June 23, **2019**.
- 37. Dequan Xiao**, "Ligand design for Parkinson's disease and Leukemia cancer studies by integrating computational chemistry and experimental approaches", ACS New Haven Local Section Meeting, New Haven, February 13, **2019**.
- 36. Dequan Xiao**, "Inverse Molecular Design of Green Catalysts for Converting Biomass into Value-Added Chemicals", Chemistry Seminar at Brown University, February 1st, **2019**.
- 35. Dequan Xiao**, "Inhibitor design for the UCHL1 enzyme by integrating computational chemistry and experimental approaches", Biochemistry Seminar at Wesleyan University, October 1st, **2018**.
- 34. Dequan Xiao**, "Inverse Molecular Design Theory and Electron Transfer in Catalysis", Seminar at Southern University of Science and Technology (Shenzhen, China), July 3, **2018**.
- 33. Dequan Xiao**, "Inverse Molecular Design Theory and Electron Transfer in Catalysis", Seminar at South China University of Technology (Guangzhou, China), July 2, **2018**.
- 32. Dequan Xiao**, "Inverse Molecular Design Theory and Electron Transfer in Catalysis", Seminar at Central South University (Changsha, China), June 28, **2018**.
- 31. Dequan Xiao**, "Inverse Molecular Design Theory and Electron Transfer in Catalysis", Seminar at Peking University (Beijing, China), June 27, **2018**.
- 30. Dequan Xiao**, "Inverse Molecular Design Theory and Electron Transfer in Catalysis", Seminar at Beijing Normal University (Beijing, China), June 26, **2018**.
- 29. Dequan Xiao**, "Inverse Molecular Design Theory and Electron Transfer in Catalysis", Seminar at ShanghaiTech University (Shanghai, China), June 24, **2018**.
- 28. Dequan Xiao**, "Inverse Molecular Design Theory and Electron Transfer in Catalysis", Seminar at Shanghai University for Science and Technology (Shanghai, China), June 24, **2018**.
- 27. Dequan Xiao**, "Inverse Molecular Design Theory in Catalysis and Ab Initio Quantum Chemistry Simulations of Vibrational SFG Spectra", Seminar at Fudan University (Shanghai, China), June 15, **2018**.
- 26. Dequan Xiao**, "Inverse Molecular Design Theory and Electron Transfer in Catalysis", Seminar at Nanjing University (Nanjing, China), June 14, **2018**.
- 25. Dequan Xiao**, "De Novo Design of Molecular Inhibitors for Parkinson's Disease Study and Fabrication of Photo-Deformable Polymer Nanospheres", ACS Student Club Seminar, University of New Haven, October 5, **2017**.
- 24. Dequan Xiao**, "De Novo Design of Molecular Inhibitors for Parkinson's Disease Study and Fabrication of Photo-Deformable Polymer Nanospheres", Biomedical Engineering Seminar, University of New Haven, October 5, **2017**.
- 23. Dequan Xiao**, "Designing Heterogeneous Catalysts for Biomass Conversion: Inverse Molecular Design and Orbital-Specific Binding Energy Analysis", 1st New England Energy Research Forum "Materials and Processes for Clean Energy", Worcester Polytechnic Institute, June 27, **2017**.
- 22. Dequan Xiao**, "Drive the Discovery of Green Catalysts for Biomass Conversion Using Inverse Molecular Design Approaches", Chemistry Department Seminar, Shenzhen University (Shenzhen, China), June 19, **2017**.

- 21. Dequan Xiao**, “Drive the Discovery of Green Catalysts for Biomass Conversion Using Inverse Molecular Design Approaches”, Chemistry College Seminar, Sichuan University (Chengdu, China), June 14, **2017**.
- 20. Dequan Xiao**, “Optimizing Catalytic Surfaces of Earth-Abundant Metals for Biomass Conversion Using the Inverse Molecular Design Approach”, 252nd ACS National Meeting and Exposition, Philadelphia, PA, August 21-25, **2016**.
- 19. Dequan Xiao**, “Drive the Discovery of Green Catalysts for Biomass Conversion Using Inverse Molecular Design”, The Marvin K. Peterson Library Faculty Lecture Series, University of New Haven, March 29, **2016**.
- 18. Dequan Xiao**, “Drive the Discovery of Green Catalysts for Biomass Conversion Using Inverse Molecular Design Approaches”, New England Catalysis Society Spring Meeting, Brown University, Rhode Island, May 20, **2016**.
- 17. Dequan Xiao**, “Inverse Molecular Design of Green Catalysts for Converting Biomass Molecules into Value-Added Chemicals”, 20th Annual Green Chemistry & Engineering Conference, Portland, Oregon, June 14-16, **2016**.
- 16. Dequan Xiao**, “Drive the Discovery of Green Catalysts for Biomass Conversion Using Inverse Molecular Design”, Department of Chemical Engineering Seminar, University of Rhode Island, February 18, **2016**.
- 15. Dequan Xiao**, “Prologue of Inverse Molecular Design of Green Catalysts for Biomass Conversion”, Physical Chemistry Club Seminar, Yale University, February 16, **2016**.
- 14. Dequan Xiao**, “Discovery of New Green Catalysts for Biomass Conversion Using Inverse Molecular Design”, Fall Seminar, Department of Chemistry and Environmental Science, New Jersey Institute of Technology, Newark, NJ, September 23, **2015**.
- 13. Dequan Xiao**, “Exploring the Mildest Conditions for the Design of Hydrogenation and Hydrogenolysis Catalysts”, 250th ACS National Meeting and Exposition, Boston, MA, August 16-20, **2015**.
- 12. Dequan Xiao**, “Exploring the Mildest Thermodynamic Conditions for the Inverse Design of Hydrogenation Catalysts”, 2nd International Summit on Past and Present Research Systems of Green Chemistry, Orlando, FL, September 14-16, **2015**.
- 11. Dequan Xiao**, “Toward the Inverse Molecular Design of Green Catalysts” (Invited Workshop), 1st International Summit on Past and Present Research Systems of Green Chemistry, Philadelphia, PA, August 25-27, **2014**.
- 10. Dequan Xiao**, “Inverse Molecular Design of Green Catalysts for Biomass Conversion” (Invited Talk), 1st International Summit on Past and Present Research Systems of Green Chemistry, Philadelphia, PA, August 25-27, **2014**.
- 9. Dequan Xiao**, “Inverse Molecular Design of Green Catalysts for Converting Lignocellulosic Biomass into Liquid Fuels”, 248th ACS National Meeting and Exposition, San Francisco, CA, August 10-14, **2014**.
- 8. Dequan Xiao** and Victor S. Batista, “DC-SFG, a Divide-and-Conquer Simulation of Sum Frequency Generation Spectra”, Gordon Research Conference – Vibrational Spectroscopy, University of New England, Maine, August 5-10, **2012**. (A shared talk with Victor S. Batista.)
- 7. Dequan Xiao**, Li Fu, Elsa C. Y. Yan, and Victor S. Batista, “Ab Initio Simulations of Chiral Sum Frequency Generation Spectra of Amyloid Proteins at Water/Membrane Interfaces”, 242th American Chemical Society National Meeting & Exposition, Denver, CO, August 28-Sept 1, **2011**.

6. **Dequan Xiao**, "Inverse Molecular Design for Dye-Sensitized Solar Cells", New York Theoretical and Computational Chemistry Conference, January 14, **2011**.
 5. **Dequan Xiao**, Robert C. Snoeberger III, Lauren A. Martini, Robert H. Crabtree, and Victor S. Batista, "Inverse Design of Molecular Chromophores for Dye-Sensitized Solar Cells", 240th American Chemical Society National Meeting & Exposition, Boston, MA, August 22-26, **2010**.
 4. **Dequan Xiao**, Robert C. Snoeberger III, and Victor S. Batista, "Inverse Design of Molecular Chromophores for Dye-Sensitized Solar Cells", Connecticut Quantum Chemistry Meeting at Yale University, January 22, **2010**.
 3. **Dequan Xiao**, Kunhua Lin, Qiang Fu, and Qinjian Yin, "Polymeric Nanocomposite Comprising Size-Controlled Organic Nanostructures via Copolymer-Directed Self-Assembly", American Physical Society March Meeting, Pittsburgh, PA, March 16-20, **2009**.
 2. **Dequan Xiao**, Weitao Yang, and David N. Beratan, "Inverse Molecular Design in a Tight-Binding Framework", American Physical Society March Meeting, New Orleans, LA, March 10-14, **2008**.
 1. **Dequan Xiao**, Weitao Yang, and David N. Beratan, "Inverse Molecular Design for Nonlinear Optical Materials", DARPA Predicting Real Optimized Materials (PROM) Program Review Meeting, San Francisco, CA, March 8-9, **2005**.
- **Conference posters**
 21. Stanley Menacherry, Johnny Chang, Ho-Yin Lo, and **Dequan Xiao**, "Identification of Value-Added Chemicals in Biofuels Produced by a Designed Green Catalyst Using GC-MS Techniques", Proceedings of 9th Edition of International Conference on Biofuels and Bioenergy, Arch. Chem. Res. **2018**, Volume 2, DOI: 10.21767/2572-4657-C1-003.
 20. **Dequan Xiao**, "Inverse Molecular Design of Green Catalysts for Lignin Conversion", Gordon Research Conference – Lignin, Stonehill College, MA, August 5 - 10, **2018**.
 19. **Dequan Xiao**, "Designing Green Catalysts for Biomass Conversion using Inverse Molecular Design Approaches", ASEE Summer School for Chemical Engineering Faculty, North Carolina State University, July 28-August 03, **2017**.
 18. **Dequan Xiao**, "Inverse Molecular Design of Green Catalysts for Hydrogenation and Hydrogenolysis of Biomass Molecules", Gordon Research Conference – Green Chemistry, Stowe, VT, July 31-August 05, **2016**.
 17. Jason An, and **Dequan Xiao**, "De novo Design of Inhibitors for Ubiquitin C-Terminal Hydrolases", 20th Annual Green Chemistry & Engineering Conference, Portland, Oregon, June 14-16, **2016**.
 16. Jason An, and **Dequan Xiao**, "Investigating the Binding Interactions between Ubiquitin C-Terminal Hydrolases and Inhibitors", 251th American Chemical Society National Meeting and Exposition, San Diego, CA, March 13-17, **2016**.
 15. Jason An, and **Dequan Xiao**, "Investigating the Binding Interactions between Ubiquitin C-Terminal Hydrolases and Inhibitors", Unite For Sight 13th Annual Global Health & Innovation Conference, Yale University, New Haven, CT, April 16-17, **2016**.
 14. Jason An, Armand Sebastian, Jun Lu, and **Dequan Xiao**, "Protein-DNA Interactions in Malfunctional Transcription by Molecular Dynamic Simulation", 250th American Chemical Society National Meeting and Exposition, Boston, MA August 16-20, **2015**.

13. Joseph Daou, and **Dequan Xiao**, "Understanding Protein-RNA Interactions for Alternative Splicing During Gene Expression using Molecular Dynamic Simulations", 248th ACS National Meeting and Exposition, San Francisco, CA, August 10-14, **2014**.
12. **Dequan Xiao**, Robert Crabtree, and Victor S. Batista, "Inverse Design of Catalysts for CO/CO₂ Fuel Cells", 244th American Chemical Society National Meeting & Exposition, Philadelphia, PA, August 19, **2012**.
11. **Dequan Xiao** and Victor S. Batista, "Studies of Proteins and Catalytic Systems at Interfaces: DC-SFG, a Divide-and-Conquer Simulation of Sum Frequency Generation Spectra", Gordon Research Conference – Vibrational Spectroscopy, University of New England, Maine, August 5-10, **2012**.
10. **Dequan Xiao**, Robert Crabtree, and Victor S. Batista, "Inverse Design of Catalysts for CO/CO₂ Fuel Cells", Gordon Research Conference – Fuel Cells, Bryant University, RI, August 5-10, **2012**.
9. **Dequan Xiao**, Robert C. Snoeberger III, Lauren A. Martini, Robert H. Crabtree, and Victor S. Batista, "Inverse Design of Molecular Chromophores for Dye-Sensitized Solar Cells", Yale Climate & Energy Spring Symposium, March 27, **2010**.
8. **Dequan Xiao**, "Inelastic Charge Transfer in a Molecular Interferometer", Annual Meeting of Southeastern Theoretical Chemistry Association at Duke University, Durham, NC, May 15-16, **2009**.
7. **Dequan Xiao**, Spiros S. Skourtis, Igor V. Rubtsov, and David N. Beratan, "Controlling Charge Flow with Vibronic Pathways in A Molecular Interferometer", 237th American Chemical Society National Meeting & Exposition, Salt Lake City, UT, March 22-26, **2009**.
6. **Dequan Xiao**, Spiros S. Skourtis, Igor V. Rubtsov and David N. Beratan, "Turning Charge Transfer On and Off Using Vibronic Coupling Pathways", Symposium on Securing Our Energy Future: Next Generation Photovoltaics and Solar Energies, University of North Carolina—Chapel Hill, January 15-17, **2009**.
5. **Dequan Xiao**, Spiros S. Skourtis, Igor V. Rubtsov and David N. Beratan, "IR-Controlled Tunneling Pathways. A Molecular Analog of the Double-Slit Experiment", 237th American Chemical Society National Meeting & Exposition, Salt Lake City, UT, March 22-26, **2009**.
4. Spiros S. Skourtis, **Dequan Xiao** and David N. Beratan, "Controlled Charge-Flow in A Molecular Interferometer", American Physical Society March Meeting, New Orleans, LA, March 10-14, **2008**.
3. Xiangqian Hu, **Dequan Xiao**, Shahar Keinan, Weitao Yang, Michael J. Therien, Koen Clays and David N. Beratan, "Understanding and Predicting the Frequency Dependent First-Hyperpolarizabilities Based on Linear Absorption Spectra and Generalized Sum Rules", Symposium on Photonics at the Frontiers of Science and Technology (Fitzpatrick Institute for Photonics 8th Annual Meeting), Durham, NC, October 13-14, **2008**.
2. Xiangqian Hu, **Dequan Xiao**, Weitao Yang, and David N. Beratan, "Inverse Design for Nonlinear Optical Materials by the Linear Combination of Atomic Potentials (LCAP) Method", Symposium on Photonics at the Frontiers of Science and Technology (Fitzpatrick Institute for Photonics 6th Annual Meeting), Durham, NC, September 28-29, **2006**.
1. **Dequan Xiao**, Weitao Yang, and David N. Beratan, "Inverse Molecular Design for Nonlinear Optical Materials", DARPA Predicting Real Optimized Materials (PROM) Program Review Meeting, San Francisco, CA, March 8-9, **2005**.