

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

Associate Professor: September 2019 --

Assistant Professor: August 2013 – August 2019

Yale University, Department of Chemistry

Associate Research Scientist: May 2012 – July 2013

Postdoctoral Research Associate: August 2009 – April 2012

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

17. PI, Industrial contract, \$15,000, 01/2020-07/2020

Title: "Computational Analysis of Protein-Ligand Interactions for Drug Discovery"

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: "Building up the Higasket Polymer Materials Laboratory"

8. Co-PI, a team proposal awarded by Connecticut BioInnovative 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
- Basics of Computational Chemistry
- 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, Physical Chemistry Chemical Physics, 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 (USA), NASA CT Space Grant Consortium, National Science Centre (Poland)
- **Advisory Board Member:**
NASA Connecticut Space Grant Consortium
- **Educational Programs Developer:**
One of the founding faculty of the new Biomedical Engineering MS program at the University of New Haven in 2014
Original developer for the new chemistry MS program (based on the *integrative approach*) at the University of New Haven in 2017

PUBLICATIONS

According to Google Scholar in **November, 2020**, total number of citations: **1730**, h-index: **24**

- **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

70. Jiliang Ma, Yancong Li, Hang Su, Dongnv Jin, Gaojie Jiao, **Dequan Xiao**, and Runcang Sun "Highly Selective Oxidation of Biomass Derivatives by Ultrahigh-Loading of Single-Atoms in Photocatalysts", *Manuscript*, **2020**, submitted.
69. Mi Peng, Chunyang Dong, Rui Gao, **Dequan Xiao**, Hongyang Liu, and Ding Ma "Fully-Exposed Cluster Catalyst: Towards Rich Surface Sites and Full Atom Utilization Efficiency", *Manuscript*, **2020**, submitted.
68. Jing-he Yang, Mi Peng, Dan-Dan Zhai, **Dequan Xiao**, Zhang-Jie Shi, Siyu Yao, and Ding Ma, "Direct Fixation of N₂ into Value-Added Organic Chemicals", *Manuscript*, **2020**, submitted.
67. Danielle S. Hanson, Yigui Wang, Xinrui Zhou, Erik Washburn, Merve B. Ekmekci, Donovan Dennis, Amay Paripati, **Dequan Xiao**, and Meng Zhou "An Experimental and Computational Study of the Catalytic Formation of Urea from Ammonium Carbamate Using A Copper(II) Complex", *Manuscript*, **2020**, submitted.
66. Michael Orsini, Johnny Chang, Laurene Petitjean, David Landofi, William Schwartz, Lin Zhang, Zhaohui Tong, Paul T. Anastas, and **Dequan Xiao**, "Designing Heterogeneous Catalysts for Lignin Degradation Guided by Inverse Molecular Design Theory", *Manuscript*, **2020**, submitted.
65. Pashupati Pokharel, Feng Wei, and **Dequan Xiao**, "Thermomechanical Properties of Polypropylene and Styrene-Ethylene-Butylene-Styrene Blends: A Molecular Dynamics Simulation and Experimental Study", *Manuscript*, **2020**, submitted.
64. Deval Prasad Bhattarai, Pashupati Pokharel, and **Dequan Xiao**, "Surface Functionalization of Polymers", *Book Chapter* in Gutierrez T. J. (eds), *Reactive and Functional Polymers Volume Four*, Springer, Cham. **2020**.
63. Lawrence M Pratt, Jihyun Kim, Ho-Yin Lo, Dequan Xiao, "Brown Grease Pyrolysis under Pressure: Extending the Range of Reaction Conditions and Hydrocarbon Product Distributions", *Fuel*, **2020**, accepted. (IF=5.1)
62. Xiao Zhang, Yang Liu, Mengtao Zhang, Tao Yu, Bingbing Chen, Yao Xu, Mark Crocker, Xiaobing Zhu, Yuchen Zhu, Rongming Wang, **Dequan Xiao**, Mingshu Bi, Ding Ma, Chuan Shi "Synergy Between Beta-Mo₂C Nanorods and Non-Thermal Plasma for Selective CO₂ Reduction to CO", *Chem*, **2020**, online. (IF=11.5)
61. Hanxi Bao, William J. Sagues, Yigui Wang, Shunchang Yang, **Dequan Xiao**, and Zhaohui Tong, "Depolymerization of Lignin to Monophenolics by Ferrous/Persulfate Reagent Under Mild Conditions", *ChemSusChem*, **2020**, accepted. (IF=8.0)
60. 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", *Nano Research*, **2020**, online. (IF=8.2)
59. Chunyang Dong, Yinlong Li, Danyang Cheng, Mengtao Zhang, Jinjia Liu, Yang-Gang Wang, Dequan Xiao, and Ding Ma "Supported Metal Clusters: Fabrication and Applications in Heterogeneous Catalysis", *ACS Catalysis*, **10**, **2020**, 19, 11011-11045. (IF=12.4)
58. 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", *Applied Catalysis. B: Environmental*, **2020**, in press. (IF=16.7)
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**, and Ding Ma "Photothermal Conversion of CO₂ with Tunable Selectivity

Using Iron-Based Catalysts: From Oxide to Carbide", *ACS Catalysis*, 10, 2020, 10364-10374. (IF=12.4)

56. Jijiao Zeng, Zhaohui Tong, Hanxi Bao, Nusheng Chen, Fei Wang, Yigui Wang, and **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. (IF=7.7)

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=2.6)

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=12.1)

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=14.6)

49. Siwei Li, Jinghe Yang, Chuqiao Song, Qingjun Zhu, and **Dequan Xiao**, Ding Ma "Iron Carbides: Control Synthesis and Catalytic Applications in CO_x Hydrogenation and Electrochemical HER" *Advanced Materials*, 2019, 1901796. (IF=27.4)

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=12.1)

47. Pengqi Yan, Wenhan Guo, Zibin Liang, Wei Meng, Zhen Yin, Siwei Li, Mengzhu Li, Mengtao Zhang, Jie Yan, **Dequan Xiao**, Ruqiang Zou, and Ding Ma "Highly Efficient K-Fe/C Catalysts Derived From Metal-Organic Frameworks Towards Ammonia Synthesis" *Nano Research*, 2019, 1-7. (IF=8.2)

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=12.4)

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=12.1)

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=12.4)

43. Pashuapati 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=7.6)

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 Selective Synthesis of Biomass-Derived D-xylonic Acid via Regulation of Structure Effect" *Green Chemistry*, 20, 2018, 5188-5195. (IF=9.4)

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*, 4, 2018, 2493-2495. (IF=11.5)

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=14.6)

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=5.0)

38. Yueshen Wu, Benjamin Rudsteyn, 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=2.3)

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=7.6)

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=9.4)

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=13.0)

32. Aimin Ge, Benjamin Rudsteyn, Brian T. Psciuk, **Dequan Xiao**, Jia Song, Chantelle L. Anfuso, 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=4.2)

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=6.7)

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 Koeppe, 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=2.6)

2014

27. Cheng Jin, Taoran Zhang, Lingyu Wang, Meiying 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, Fangzhuan 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=3.1)

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=2.6)

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=14.6)

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=3.7)

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=13.0)

2012

20. Xuewen 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=3.1)

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=2.5)

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=2.5)

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=5.1)

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=4.2)

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=14.6)

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=14.6)

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=2.6)

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=2.6)

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.

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=0.8)

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=4.2)

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=4.1)

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=21.7)

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=12.3)

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- 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**.
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- 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**.
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