

## Dequan Xiao, Ph. D.

Assistant Professor, University Research Scholar  
Director, Center for Integrative Materials Discovery  
Director, HIGA Polymer Materials Laboratory  
Campus Director, NASA Connecticut Space Grant Consortium  
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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

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### EMPLOYMENT HISTORY

**University of New Haven, Department of Chemistry and Chemical Engineering**  
Assistant Professor: August 2013 -- Present

**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

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## AWARDS AND HONORS

- 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

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## GRANT AWARDS

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 a 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"

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## PROFESSIONAL MEMBERSHIPS

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

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## COURSE TEACHING

### University of New Haven

- Physical Chemistry
- Physical Chemistry Laboratory
- Introduction to Computational Chemistry
- Polymer Science

### 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

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## ACADEMIC SERVICES

- **Journal Reviewer:**  
Journal of American Chemical Society, Journal of Physical Chemistry Letters, Journal of Physical Chemistry, Journal of Materials Chemistry, RSC Advances, Journal of Applied Polymer Science, Journal of Molecular Modeling, Molecules, Journal of Mathematical Bioscience, Computational and Theoretical Chemistry, the Korean Journal of Chemical Engineering, Nature-Scientific Data, RSC Open Science, Sensors & Actuators: B. Chemical, Computing in Science and Engineering, Journal of Chemical Theory and

Computation, Solid-State Ionics, Journal of Inorganic Biochemistry, ACS Omega, Catalysts, Applied Science

- **Grant Reviewer:**  
NSF (USA), NASA CT Space Grant Consortium, National Science Centre (Poland)
- **Advisory Board:**  
NASA Connecticut Space Grant Consortium
- **Educational Programs:**  
One of the founding faculties of the new Biomedical Engineering MS program at the University of New Haven in 2014  
Developed a new chemistry-MS program proposal at the University of New Haven in 2017

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## PUBLICATIONS

According to Google Scholar in August, 2018, total number of citations: 1002, h-index: 18

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

## Chemical Theories: Inverse Molecular Design Theory, Charge Transfer Theory, Nonlinear Optics Theory, and Vibrational Sum Frequency Generation Simulation

**13. 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.

**12.** 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=2.8)

**11.** 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)

**10. 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.

**9.** 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)

**8. 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 TiO<sub>2</sub> Sensitization", *Journal of American Chemical Society*, **133**(23), **2011**, 9014-9022. (IF=14.4)

**7.** 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)
6. 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)
5. 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)
4. 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)
3. 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)
2. 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)
1. 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)

## Catalysis

13. Jiliang Ma, Zewei Liu, Junlong Song, Linxin Zhong, Dequan Xiao, Hongxia Xi, Xuehui Li, Run-Cang Sun and Xinwen Peng, "Au@h-Al<sub>2</sub>O<sub>3</sub> analogic yolk-shell nanocatalyst for highly selectively synthesis of biomass-derived D-xylonic acid via regulation of structure effect" *Green Chemistry*, 2018, just accepted. (IF=8.6)
12. 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)*, 2018, just accepted. (IF=14.1)
11. 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*, 2018, Article ASAP. (IF=14.4)
10. 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 TiO<sub>2</sub> Nanoparticles under Visible Light Irradiation" *International Journal of Hydrogen Energy*, 43(9), 2018, 4335-4346. (IF=4.2)
9. Yueshen Wu, Benjamin Rudshteyn, Ingolf Warnke, Dequan Xiao, Victor S. Batista, "Mechanistic study of CO/CO<sub>2</sub> conversion catalyzed by a biomimetic Ni(II)-iminothiolate complex", *International Journal of Quantum Chemistry*, 118, 2018, e25555. (IF=2.6)
8. Dequan Xiao and Trevor Callahan, "The role of atomic orbitals of doped earth-abundant metals on designed copper catalytic surfaces", 2017, arXiv:1701.04333.
7. 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)

6. 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)

5. 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 CO<sub>2</sub>-Reduction Catalyst on Rutile TiO<sub>2</sub>(110) Surfaces", **Journal of Physical Chemistry C**, 120(37), 2016, 20970-20977. (IF=4.5)

4. 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)

3. **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. Mammìno, Royal Society of Chemistry, Cambridge, 978-1-84973-949-8, 2015.

2. Chantelle L. Anfuso, **Dequan Xiao**, Allen M. Ricks, Christian F. A. Negre, Victor S. Batista, and Tianquan Lian, "Orientation of a Series of CO<sub>2</sub> Reduction Catalysts on Single Crystal TiO<sub>2</sub> Using Phase-Sensitive Vibrational Sum Frequency Generation Spectroscopy (PS-VSFGS)", **Journal of Physical Chemistry C**, 116(45), 2012, 24107-24114. (IF=4.5)

1. Chantelle Anfuso, Robert C. Snoeberger III, Allen Ricks, Weimin Liu, **Dequan Xiao**, Victor S. Batista, and Tianquan Lian, "Covalent Attachment of a Rhenium Bipyridyl CO<sub>2</sub> Reduction Catalyst to Rutile TiO<sub>2</sub>", **Journal of American Chemical Society**, 133(18), 2011, 6922-6925. (IF=14.4)

## Biomolecules

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

4. 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)

3. 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)

2. **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)

1. 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)

## Polymers Materials

11. 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)

**10.** Cheng Jin, Taoran Zhang, Lingyu Wang, Meiyang 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)

**9.** Cheng Jin, Taoran Zhang, Fangzhan 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)

**8.** 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=2.9)

**7.** 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)

**6.** 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)

**5.** 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)

**4.** 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)

**3.** 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)

**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**

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”, 252<sup>nd</sup> 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”, 20<sup>th</sup> 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”, 250<sup>th</sup> 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”, 2<sup>nd</sup> 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), 1<sup>st</sup> 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), 1<sup>st</sup> 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”, 248<sup>th</sup> 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”, 242<sup>th</sup> 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”, 240<sup>th</sup> 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**

**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**.

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