

## **Dequan Xiao, Ph. D.**

Assistant Professor

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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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### **ACADEMIC EMPLOYMENT**

#### **University of New Haven, Department of Chemistry and Chemical Engineering**

Assistant Professor: August 2013 -- Present

#### **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

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### **AWARDS AND HONORS**

- University Research Scholar, 2016. (An award to 3-4 research-active faculties per year at the University of New Haven.)
- Project Award by Yale PITCH Program, 2015. (An award to selected projects for conducting translational research on pre-drug discovery, supported by Connecticut State BioInnovative Program.)

- Conference Travel Fellowship, 2008. (An award to qualified graduate student applicants at Duke University.)
- PLU Travel Grant, 2008. (An award to top three graduate student applicants in the Chemistry Department of Duke University.)
- University Merit Fellowship, 2002. (An award to 2 out of all (~20) graduate students in the Chemistry Department at UCF.)
- Procter & Gamble Outstanding Graduate Student Scholarship, 1998. (An award to 2 students out of all graduate students (~500) at Sichuan University.)
- Admitted into the M.S. graduate program of Sichuan University with the exemption of standardized national entrance exams due to the academic excellence, 1996. (An honor to the top 5% of students out of 150 undergraduates in the Chemistry Department of Sichuan University.)
- Annual Academic Excellence Scholarship, 1993, 1994, 1995, 1996, respectively. (Awards to top 5% of undergraduates in the Chemistry Department of Sichuan University.)
- Excellence Prize in Chemistry Olympic Match (for High School Students), Guangdong Province, 1991.

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## GRANT AWARDS

**11.** PI, University Research Scholar Research Fund, University of New Haven, \$12,000, 05/2016-04/2019

**10.** PI, Summer Research Grant and Research Fund, University of New Haven, \$5,250, 07/2016-06/2017

**9.** PI, Research donation fund from Higasket Plastics Group Co. Ltd., \$100,000, 06/2016-05/2021.

**8.** Co-PI, a team proposal awarded by Connecticut BioInovative 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.** Key consultant, 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
- **Grant Reviewer:**  
NSF Proposals, NASA CT Space Grants
- **Advisory Board:**  
NASA Connecticut Space Grant Consortium

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## PUBLICATIONS

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

- **Peer-reviewed articles**

**2016**

36. Weixin Huang, Shiran Zhang, Yu Tang, Yuting Li, Luan Nguyen, Yuanyuan Li, Junjun Shan, **Dequan Xiao**, Raphael Gagne, Anatoly I. Frenkel, Franklin (Feng) Tao, "Low-Temperature Transformation of Methane to Methanol on Pd<sub>1</sub>O<sub>4</sub> Single Sites Anchored on the Internal Surface of Microporous Silicate", *Angew. Chem. Int. Ed.*, **2016**, *in press*.

35. Raphael Gagne, Laurene Petitjeana, Evan S. Beach, Jason An, Paul T. Anastas, and **Dequan Xiao**, "Exploring the Mildest Conditions for the Hydrogenation and Hydrogenolysis of Functional Groups in Lignin Biomass", Manuscript, **2016**, submitted.

34. **Dequan Xiao**, Rui Hu, "A Tutorial of the Inverse Molecular Design Theory in Tight-Binding Frameworks and Its Applications", Book Chapter (invited), **2016**.

33. 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*, Article ASAP, **2016**.

32. 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.

**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.

30. 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.

29. 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.

28. **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**.

**2014**

27. 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.

26. **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.

25. 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.

24. 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.

### 2013

23. 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.

22. 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.

21. 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.

### 2012

20. 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-VSFG)", *Journal of Physical Chemistry C*, 116(45), **2012**, 24107-24114.

19. **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.

18. 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.

17. 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.

16. 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.

## 2011

15. **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.

14. 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.

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.

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.

## 2010

11. 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.

10. 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.

9. 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.

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.

## 2009

7. 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.

6. 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.

5. **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.

#### 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.

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.

#### 2002

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.

#### 2000

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**

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, PA, September 14-16, **2015**.
- 11. Dequan Xiao**, "Toward the Inverse Molecular Design of Green Catalysts" (Invited Workshop), 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**

**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”, 20<sup>th</sup> 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”, 251<sup>th</sup> 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 13<sup>th</sup> 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”, 250<sup>th</sup> 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”, 248<sup>th</sup> 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/CO<sub>2</sub> Fuel Cells”, 244<sup>th</sup> 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/CO<sub>2</sub> 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”, 237<sup>th</sup> 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”, 237<sup>th</sup> 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**.