Dequan Xiao, Ph. D.

Associate Professor & Endowed Jacob F. Buckman Chair
Director, Center for Integrative Materials Discovery
Chair, Department of Chemistry and Chemical and Biomedical Engineering

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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 & Biomedical 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

20. PI, Buckman Chair Endow Professorship Award, University of New Haven, $90,000, 09/2022-08/2025

19. PI, Industry contract, $98,500, 02/2022-11/2022
Title: “AI Driven Inhibitor Design for Cancer Research”

18. co-PI, DOE-EMSL exploratory proposal award, *analysis resources and computing time support*s, 01/2022-10/2022
Title: “Characterizing Key Factors That Influence Recalcitrance of Lignocellulosic Biomass Deconstruction via *in-situ* liquid IR SNOM Approach”

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 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. 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, ACS Nano, ACS Au, ACS Catalysis, ACS Applied Materials and Interfaces, ACS Sustainable Chemistry and Engineering, Journal of Physical Chemistry Letters, Journal of Chemical Theory and Computation, Journal of Physical Chemistry, ACS Omega, Nature-Scientific Data, Nature Communications, Journal of Materials Chemistry, Physical Chemistry Chemical Physics, Biomass Conversion and Biorefinery, RSC Advances, RSC Open Science, Diamond and Related Materials, Journal of Applied Polymer Science, ChemPhotoChem, ChemCatChem, iScience, ChemoSphere, 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 Fondation (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 **December, 2022**, total number of citations: **3,723**, h-index: **34**

- **PhD dissertation**

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

- **MS Thesis**

  Dequan Xiao, "Self-assembly of polyelectrolyte-coated silver nanoparticles with metanil yellow for use in Raman amplification", University of Central Florida, **2003**.

Research Articles or Reviews

2022

105. Xiao Zhang, Yao Xu, Yang Liu, Liang Niu, Yanan Diao, Zirui Gao, Bingbing Chen, Jinglin Xie, Mingshu Bi, Meng Wang, **Dequan Xiao**, Ding Ma, and Chuan Shi, "A novel Ni–MoCxOy interfacial catalyst for syngas production via the chemical looping dry reforming of methane", **Chem**, **2022**, in press. (IF=25.8)

104. Hao-Xin Liu, Jin-Ying Li, Xuetao Qin, Chao Ma, Wei-Wei Wang, Kai Xu, Han Yan, **Dequan Xiao**, Chun-Jiang Jia, Qiang Fu and Ding Ma, "Ptn–Ov synergistic sites on MoOx/γ-Mo2N heterostructure for low-temperature reverse water–gas shift reaction", **Nature Communications**, 13, **2022**, 5800. (IF=17.7)

103. Zhimin Jia, Xuetao Qin, Yunlei Chen, Xiangbin Cai, Zirui Gao, Mi Peng, Fei Huang, **Dequan Xiao**, Xiaodong Wen, Ning Wang, Zheng Jiang, Wu Zhou, Hongyang Liu, and Ding Ma, "Fully-exposed Pt-Fe cluster for efficient preferential oxidation of CO towards hydrogen purification", **Nature Communications**, 13, **2022**, 6798. (IF=17.7)

102. Fei Huang, Mi Peng, Yunlei Chen, Xiangbin Cai, Xuetao Qin, Ning Wang, **Dequan Xiao**, Li Jin, Guoqing Wang, Xiaodong Wen, Hongyang Liu, and Ding Ma, "Low Temperature Acetylene Semi-Hydrogenation over the Pd1-Cu1 Dual-Atom Catalyst", **Journal of American Chemical Society**, 144(40), **2022**, 18485-18493. (IF=16.4)

101. Zhaohui Yin, Kun Zhang, Na Ma, Xi Liu, Zhen Yin, Hong Wang, Xue Yang, Ye Wang, Xuetao Qin, Yuchen Deng, Yumei Zheng, Lili Wang, Jianxin Li, Zongwei Xu, Na Tang, Bowen Cheng, **Dequan Xiao**, and Ding Ma, "Catalytic Membrane Electrode with Co_3O_4 Nanoarrays for Simultaneous Recovery of Water and Hydrogen Energy from Wastewater", **Science China Materials**, **2022**. (IF=8.3)

100. Danyang Cheng, Meng Wang, **Dequan Xiao**, Ding Ma, "Cu/Mo2CT interface drives CO2 hydrogenation to methanol", **Matter**, 5(8), **2022**, 2469-2471. (IF=15.6)

99. Mei-Qi Zhang, Meng Wang, Bo Sun, Chaoquan Hu, **Dequan Xiao**, and Ding Ma, "Catalytic strategies for upvaluing plastic wastes", **Chem**, 11(8), **2022**, 2912-2923. (IF=22.8)

98. Yu Guo, Maolin Wang, Qingjun Zhu, **Dequan Xiao**, Ding Ma, "Ensemble effect for single-atom, small cluster and nanoparticle catalysts", **Nature Catalysis**, 9(5), **2022**, 766-776. (IF=40.7)

97. Ruochen Cao, Mei-Qi Zhang, Chaoquan Hu, **Dequan Xiao**, Meng Wang, and Ding Ma, "Catalytic Oxidation of Polystyrene to Aromatic Oxygenates over Graphitic Carbon Nitride Catalyst", **Nature Communications**, 13, **2022**, 4809. (IF=17.7)

96. Zhimin Jia, Mi Peng, Xiangbin Cai, Yunlei Chen, Xiaowen Chen, Fei Huang, Linmin Zhao, Jiangyong Diao, Ning Wang, **Dequan Xiao**, Xiaodong Wen, Zheng Jiang, Hongyang Liu, and Ding

Ma, “Fully Exposed Platinum Clusters on Nanodiamond/Graphene Hybrid for efficient low-temperature CO oxidation”, **ACS Catalysis**, 12 (15), **2022**, 9602-9610. (IF=13.1)

95. Xian Zhou, Xiaofeng Gao, Mingjie Liu, Zirui Gao, Xuetao Qin, Wenhao Xu, Shitong Ye, Wenhua Zhou, Haoan Fan, Jing Li, Shurui Fan, Lei Yang, Jie Fu, **Dequan Xiao**, Lili Lin, Ding Ma, and Siyu Yao, “Photocatalytic Dehydrogenative C-C Coupling of Acetonitrile to Succinonitrile”, **Nature Communications**, 13, **2022**, 4379. (IF=17.7)

94. Fanchi Meng, Xuetao Qin, Lini Yang, Fei Huang, Jiangyong Diao, Xiangbin Cai, Di Zhang, ling Li, Pengbo Zhu, Mi Peng, Ning Wang, **Dequan Xiao**, Lixin Xia, Hongyang Liu, and Ding Ma, “Fully-exposed Pd cluster catalyst: an excellent catalytic antibacterial nanomaterial”, **Small**, 18(33), **2022**, 2203283. (IF=15.2)

93. Mi Peng, **Dequan Xiao**, and Ding Ma, “Envisioning Quantitative Catalytic Superiority of Interfacial Sites in Three Dimensions”, **Chem**, *8(4)*, **2022**, 892-894.

92. Fei Huang, Mi Peng, Yunlei Chen, Zirui Gao, Xiangbin Cai, Jinglin Xie, **Dequan Xiao**, Li Jin, Guoqing Wang, Xiaodong Wen, Ning Wang, Wu Zhou, Hongyang Liu, and Ding Ma, “Insight into the Activity of Atomically Dispersed Cu Catalysts for Semihydrogenation of Acetylene: Impact of Coordination Environments”, **ACS Catalysis**, *12(1)*, **2022**, 48-57. (IF=13.1)

91. Jiliang Ma, Yancong Li, Hang Su, Dongnv Jin, Gaojie Jiao, Hang Su, **Dequan Xiao**, Runcang Sun "Single-atom zinc catalyst for co-production of hydrogen and fine chemicals over soluble biomass solution", **Advanced Powder Materials**, **2022**, 100058.

90. Danyang Cheng, Meng Wang, Lipeng Tang, Zirui Gao, Xuetao Qin, Yongjun Gao, **Dequan Xiao**, Wu Zhou, Ding Ma, "Catalytic Synthesis of Formamides by Integrating CO2 Capture and Morpholine Formylation on Supported Iridium Catalyst", **Angewandte Chemie**, **2022**, e202202654. (IF=16.8)

89. Fubo Gu, Xuetao Qin, Mengwei Li, Yao Xu, Song Hong, Mengyao Ouyang, Georgios Giannakakis, Sufeng Cao, Mi Peng, Jinling Xie, Meng Wang, Dongmei Han, **Dequan Xiao**, Xiayan Wang, Zhihua Wang, Ding Ma, "Selective Catalytic Oxidation of Methane to Methanol in Aqueous Medium over Copper Cations Promoted by Atomically Dispersed Rhodium on TiO2", **Angewandte Chemie**, 61(18), **2022**, e202201540. (IF=16.8)

88. Linmin Zhao, Xuetao Qin, Xirui Zhang, Xiangbin Cai, Fei Huang, Zhimin Jia, Jiangyong Diao, **Dequan Xiao**, Zheng Jiang, Ruifeng Lu, Ning Wang, Hongyang Liu, Ding Ma, "A Magnetically Separable Pd Single-Atom Catalyst for Efficient Selective Hydrogenation of Phenylacetylene", **Advanced Materials**, 34(20), **2022**, 2110455. (IF=32.1)

87. Jing-He Yang, Mi Peng, Dan-Dan Zhai, **Dequan Xiao**, Zhang-Jie Shi, Siyu Yao, Ding Ma, "Fixation of N2 into Value-Added Organic Chemicals", **ACS Catalysis**, 12(5), **2022**, 2898-2906. (IF=13.1)

86. Yang Liu, Yong Chen, Zirui Gao, Xiao Zhang, Lejian Zhang, Meng Wang, Bingbing Chen, Yanan Diao, Yilong Li, **Dequan Xiao**, Xinping Wang, Ding Ma, ChuanShi, "Embedding high loading and uniform Ni nanoparticles into silicalite-1 zeolite for dry reforming of methane", **Applied Catalysis B: Environmental**, 307(15), **2022**, 121202. (IF=21.4)

85. FanChi Meng, Mi Peng, Yunlei Chen, Xiangbin Cai, Fei Huang, Lini Yang, Xiao Liu, Tao Li, Xiaodong Wen, Ning Wang, **Dequan Xiao**, Hong Jiang, Lixin Xia, Hongyang Liu, Ding Ma, "Defect-rich graphene stabilized atomically dispersed Cu3 clusters with enhanced oxidase-like activity for antibacterial applications", **Applied Catalysis B: Environmental**, 301, **2022**, 120826. (IF=21.4)

84. Mi Peng, Zhimin Jia, Zirui Gao, Ming Xu, Danyang Cheng, Meng Wang, Chengyu Li, Linlin Wang, Xiangbin Cai, Zheng Jiang, Hong Jiang, Ning Wang, **Dequan Xiao**, Hongyang Liu, and Ding Ma,

"Antisintering Pd1 Catalyst for Propane Direct Dehydrogenation with In Situ Active Sites Regeneration Ability", **ACS Catalysis**, 12(4), **2022**, 2244-2252. (IF=13.1)

83. Yinwen Li, Meng Wang, Xingwu Liu, Chaoquan Hu, **Dequan Xiao**, and Ding Ma, "Catalytic Transformation of PET and CO2 into High-Value Chemicals ", **Angewandte Chmie**, 134(10), **2022**, e202117205. (IF=16.8)

2021

82. Fei Huang, Mi Peng, Yunlei Chen, Zirui Gao, Xiangbin Cai, Jinglin Xie, **Dequan Xiao**, Li Jin, Guoqing Wang, Xiaodong Wen, Ning Wang, Wu Zhou, Hongyang Liu, Ding Ma, "Insight into the Activity of Atomically Dispersed Cu Catalysts for Semihydrogenation of Acetylene: Impact of Coordination Environments", **ACS Catalysis**, 12(1), **2021**, 48-57. (IF=13.1)

81. Zhibo Liu, Fei Huang, Mi Peng, Yunlei Chen, Xiangbin Cai, Linlin Wang, Zenan Hu, Xiaodong Wen, Ning Wang, **Dequan Xiao**, Hong Jiang, Hongbin Sun, Hongyang Liu, Ding Ma, "Tuning the selectivity of catalytic nitriles hydrogenation by structure regulation in atomically dispersed Pd catalysts", **Nature Communications**, 12, **2021**, 6194. (IF=17.7)

80. Jiliang Ma, Dongnv Jin, Yancong Li, **Dequan Xiao**, Gaojie Jiao, Qiong Liu, 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**, 283, **2021**, 119520. (IF=21.4)

79. Shaopeng Li, Minghua Dong, Mi Peng, Qingqing Mei, Yanyan Wang, Junjuan Yang, Youdi Yang, Bingfeng Chen, Shulin Liu, **Dequan Xiao**, Huizhen Liu, Ding Ma, Buxing Han, "Crystal-phase engineering of PdCu nanoalloys facilitates selective hydrodeoxygenation at room temperature", **Innovation**, 3(1), **2021**, 100189.

78. Chuqiao Song, Zhaohua Wang, Zhen Yin, **Dequan Xiao**, and Ding Ma, "Principles and Applications of Photothermal Catalysis", **Chem Catalysis,** *2(1)*, **2021,** 52-83.

77. Mi Peng, **Dequan Xiao**, and Ding Ma, "An Electrified Insight into the Thermocatalysis in Water", **Joule**, *11(17)*, **2021**, 2768-2771 (online). (IF=41.2)

76. Lili Lin, Yuzhen Ge, Hongbo Zhang, Meng Wang, **Dequan Xiao**, Ding Ma, "Heterogeneous Catalysis in Water", **JACS Au**, *1(11)*, **2021**, 1834-1848. (IF=12.4)

75. Peng Zhai, Yinwen Li, Meng Wang, Jinjia Liu, Zhi Cao, Jie Zhang, Yao Xu, Xingwu Liu, Yong-Wang Li, Qingjun Zhu, **Dequan Xiao**, Xiao-Dong Wen and Ding Ma, "Development of Direct Conversion of Syngas to Unsaturated Hydrocarbons based on Fischer-Tropsch Route", **Chem**, *7(11)*, **2021**, 3027-3051. (IF=22.8)

74. Linlin Wang, Jiangyong Diao, Mi Peng, Yunlei Chen, Xiangbin Cai, Yuchen Deng, Fei Huang, Xuetao Qin, **Dequan Xiao**, Zheng Jiang, Ning Wang, Ting Sun, XiaoDong Wen, Hongyang Liu, and Ding Ma, "Cooperative Sites in Fully Exposed Pd Clusters for Low-temperature Direct Dehydrogenation Reaction", **ACS Catalysis**, *11(18),* **2021**, 11469-11477. (IF=13.1)

73. Meng Wang, **Dequan Xiao**, and Ding Ma, "Direct Observation of the Active Sites in Methane Dehydroaromatization by NMR", **Chem**, *7(6)*, **2021**, 1424-1427. (IF=22.8)

72. Mingsai Li, Lin Xin Zhong, Wei Chen, Yiming Huang, Zhongxin Chen, **Dequan Xiao**, Ren Zou, Liang Chen, Qi Hao, Zehao Liu, Runcang Sun, and Xinwen Peng, "Regulating the Electron–Hole Separation to Promote Selective Oxidation of Biomass Using ZnS@Bi2S3 Nanosheet Catalyst", **Applied Catalysis. B: Environmental**, *292*, **2021**, 120180. (IF=21.4)

71. Emily Z. Wang, Yigui Wang, and **Dequan Xiao**, "Polymer Nanocomposites for Photocatalytic Degradation and Photo-Induced Utilizations of Azo-Dyes", **Polymers**, *13(8)*, **2021**, 1215. (IF=4.3)

70. Qian Zhuang, Na Ma, Zhaohui Yin, Xue Yang, Zhen Yin, Jian Gao, Yao Xu, Zirui Gao, Hong Wang, Jianli Kang, **Dequan Xiao**, Jianxin Li, Xifei Li, Ding Ma, "Rich Surface Oxygen Vacancies of MnO2 for Enhancing Electrocatalytic Oxygen Reduction and Oxygen Evolution Reactions", **Advanced Energy and Sustainability Research**, *2*, **2021,** 2100030.

69. Xiaowen Chen, Mi Peng, Xiangbin Cai, Yunlei Chen, Zhimin Jia, Yuchen Deng, Bingbao Mei, Zheng Jiang, **Dequan Xiao**, Xiaodong Wen, Ning Wang, Hongyang Liu, and Ding Ma, "Regulating Coordination Number in Atomically Dispersed Pt Species on Defect-Rich Graphene for n-Butane Dehydrogenation Reaction", **Nature Communications**, *12*, **2021**, 2664. (IF=17.7)

68. 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", **Inorganic Chemistry**, *60(8)*, **2021**, 5573-5589. (IF=5.2)

67. B.Gopalakrishna, N.Nagaraju, Krishna Ventakesh, **Dequan Xiao**, and N.Kathyayini "Studies on the Influence of Weight Percentage of Multiwalled Carbon Nanotubes in Mn/Ni/Co Nanocomposites for Hybrid Supercapacitors", **Inorganic Chemistry Communications**, *124*, **2021**, 108371. (IF=2.5)

66. Haiping Gao, Yigui Wang, Moyosore Alfolabi, **Dequan Xiao**, and Yongsheng Chen, "Incorporation of Cellulose Nanocrystal into Graphene Oxide Membranes for Efficient Antibiotics Removal at High Nutrients Recovery", **ACS Applied Materials and Interface**, *13(12)*, **2021,** 14102-14111. (IF=10.4)

65. Lawrence M Pratt, Jihyun Kim, Ho-Yin Lo, and **Dequan Xiao**, "Brown Grease Pyrolysis under Pressure: Extending the Range of Reaction Conditions and Hydrocarbon Product Distributions", **Fuel**, *289*, **2021**, 119782. (IF=6.6)

64. 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", **ACS Central Science**, *7(2)*, **2021**, 262-273. (IF=14.6)

63. Huizhu Cai, Bingbing Chen, Xiao Zhang, Yuchen Deng, **Dequan Xiao**, Ding Ma, and Chuan Shi, "Highly Active Sites of Low Spin FeIIN4 Species: the Identification and the ORR Performance", **Nano Research**, *14*, **2021**, 122-130. (IF=8.9)

2020

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**, *6(12)*, **2020**, 3312-3328. (IF=22.8)

61. 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**.

60. 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**, *13(24)*, **2020**, 6582-6593. (IF=9.1)

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(19)*, **2020**, 11011-11045. (IF=13.1)

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**, *283*, **2020**, 119520. (IF=21.4)

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=13.1)

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=6.6)

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=7.8)

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=3.0)

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=17.7)

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=22.4)

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=16.4)

49. Siwei Li, Jinghe Yang, Chuqiao Song, Qingjun Zhu, and **Dequan Xiao**, Ding Ma "Iron Carbides: Control Synthesis and Catalytic Applications in COx Hydrogenation and Electrochemical HER", **Advanced Materials, 2019**, 1901796. (IF=32.1)

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

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