Biographical Sketch
Zili Wu

Education/Training:

Wuhan University, Wuhan, China	B.S.	1996	Environmental Chemistry
Dalian Institute of Chemical Physics, Dalian, China.	Ph.D.	2001	Physical Chemistry
Northwestern University, Evanston, IL	Postdoc	2006	Physical Chemistry

Research and Professional Experience:

2016 – present	Group Leader of Surface Chemistry and Catalysis at ORNL
2006 – present	Research staff of Chemical Science Division and Center for Nanophase Materials Sciences, ORNL

Research Interests:

- Heterogeneous catalysis, photocatalysis electrocatalysis;
- Surface chemistry and reaction mechanisms and kinetics via *in situ/operando* spectroscopy including IR, Raman, neutron and X-ray scattering;
- Well-defined nanocatalysts including oxides, supported metals and 2D materials;
- Biomass conversion, natural gas conversion and water splitting.

Selected Publications (total > 190 including 6 book chapters, H-index = 51 (Google scholar), total citations > 9100, full publication list attached the end):

1) Zhang, X.; You, R.; Wei, Z.; Jiang, X.; Yang, J.; Pan, Y.; Wu, P.; Jia, Q.; Bao, Z.; Bai, L.; Jin, M.; Sumpter, B.; Fung, V.; Huang, W.; Wu, Z.*, Radical Chemistry and Reaction Mechanisms of Propane Oxidative Dehydrogenation over Hexagonal Boron Nitride Catalysts. *Angew. Chem. Int. Ed.* **2020,** *59*, 8042-8046
2) Moon, J.; Cheng, Y.; Daemen, L. L.; Li, M.; Polo-Garzon, F.; Ramirez-Cuesta, A. J.; Wu, Z.*, Discriminating the Role of Surface Hydride and Hydroxyl for Acetylene Semihydrogenation over Ceria through In Situ Neutron and Infrared Spectroscopy. *ACS Catal.* **2020,** *10*, 5278-5287.
3) Kammert, J.; Moon, J.; Cheng, Y.; Daemen, L.; Irle, S.; Fung, V.; Liu, J.; Page, K.; Ma, X.; Phaneuf, V.; Tong, J.; Ramirez-Cuesta, A. J.; Wu, Z.*, Nature of Reactive Hydrogen for Ammonia Synthesis over a Ru/C12A7 Electride Catalyst. *J. Amer. Chem. Soc.* **2020,** *142*, 7655-7667
4) Bao, Z.; Fung, V.; Polo-Garzon, F.; Hood, Z. D.; Cao, S.; Chi, M.; Bai, L.; Jiang, D.-e.; Wu, Z.*, The interplay between surface facet and reconstruction on isopropanol conversion over SrTiO3 nanocrystals. *J. Catal.* **2020,** *384*, 49-60.
5) Polo-Garzon, F.; Bao, Z.; Zhang, X.; Huang, W.; Wu, Z.*, Surface reconstructions of metal oxides and the consequences on catalytic chemistry. *ACS Catal.* **2019,** *9*, 5692-5707.
6) Polo-Garzon, F.; Fung, V.; Nguyen, L.; Tang, Y.; Tao, F.; Cheng, Y.; Daemen, L. L.; Ramirez-Cuesta, A. J.; Foo, G. S.; Zhu, M.; Wachs, I. E.; Jiang, D.-e.; Wu, Z.*, Elucidation of the Reaction Mechanism for High-Temperature Water Gas Shift over an Industrial-Type Copper–Chromium–Iron Oxide Catalyst. *J. Amer. Chem. Soc.* **2019,** *141*, 7900-7999.
7) Polo Garzon, F.; Fung, V.; Liu, X.; Hood, Z. D.; Bickel, E. E.; Bai, L.; Tian, H.; Foo, G. S.; Chi, M.; Jiang, D.-E.; Wu, Z. L.*, Understanding the Impact of Surface Reconstruction of Perovskite Catalysts on CH4 Activation and Combustion *ACS Catal.* **2018**, *8*, 10306.
8) Su, T.; Shao, Q.; Qin, Z.; Guo, Z.; Wu, Z.*, Role of Interfaces in Two-Dimensional Photocatalyst for Water Splitting. *ACS Catal.* **2018,** *8*, 2253-2276.

9) Polo-Garzon, F.; Wu, Z. L.*, Acid-base catalysis over perovskites: a review. *J. Mater. Chem. A* **2018,** *6*, 2877-2894.
10) Foo, G. S.; Hood, Z. D.; Wu, Z. L.*, Shape Effect Undermined by Surface Reconstruction: Ethanol Dehydrogenation over Shape-Controlled SrTiO3 Nanocrystals. *ACS Catal.* **2018,** *8*, 555-565.
11) Wu, Z.*; Cheng, Y.; Tao, F.; Daemen, L.; Foo, G. S.; Nguyen, L.; Zhang, X.; Beste, A.; Ramirez-Cuesta, A. J. J. J. o. t. A. C. S., Direct neutron spectroscopy observation of cerium hydride species on a cerium oxide catalyst. *J. Am. Chem. Soc.* **2017,** *139*, 9721-9727.
12) Polo-Garzon, F.; Yang, S.-Z.; Fung, V.; Foo, G. S.; Bickel, E. E.; Chisholm, M. F.; Jiang, D.-e.; Wu, Z.*, Controlling Reaction Selectivity through the Surface Termination of Perovskite Catalysts. *Angew. Chem. Int. Ed.* **2017,** *56* (33), 9820-9824.

Synergistic Activities:

- **PI of multiple projects** (~$4 million per year) from fundamental catalysis to applied catalysis at ORNL including DOE BES Catalysis FWP (2016 – present), EERE-AMO program (2018 - 2021) and ORNL LDRD (2018 - 2020).
- **Thrust/Theme Leader** of UNCAGE-ME Energy Research Frontier Center of DOE-BES (2014 – 2022).
- **Editorial Board**: Chinese Journal of Catalysis, 2014 – present; Chinese Chemical Letters, 2016 – present.
- **International Scientific Committee** of *3rd and 4th Fundamentals and Applications of Cerium Oxide in Catalysis*, 2018 and 2020.
- **Symposium organizers**: >15 symposia at ACS National Meetings, MRS Meeting and AVS Meeting.
- **Advisory Committees:** Northwestern University, External Advisory Board of Institute of Catalysis for Energy Processes (2017 – present)

Collaborators and Co-editors:

K. Walton, C. Jones, D. Sholl, Georgia Tech; I. Wachs, J. Baltrusatis, Lehigh University; Y. Lei, University of Alabama – Huntsville; F. Tao, University of Kansas; S.Q. Ma, University of S. Florida; W.Z. Li, University of Iowa.; S. Zhang, University of Virginia; J. Groves, Princeton University, W. Goddard, Caltech; L. Tao, NREL; H.J. Tian, University of West Virginia; S. Laursen, University of Tennessee.

Graduate and Postdoctoral Advisors and Advisees:

PhD Advisors - Qin Xin and Can Li (Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China), A. Guerrero-Ruiz (Institute of Catalysis and Petroleumchemistry, Spain);
Postdoctoral Advisor – Peter Stair (Northwestern University, USA)
Graduate Students - Mar Piernavieja-Hermida (University of Alabama – Huntsville), Lei Bai (University of West Virginia); Xiaohan Ma (Clemson University)
Postdoctoral Associates - Eric Formo (University of Georgia), Amanda Mann (Merck Inc.); Uma Tumuluri (Oak Ridge National Lab), Rui Peng (MilliporeSigma), Guo Shiou Foo (W.L. Gore & Associates), Felipe Polo Garzon (Oak Ridge National Lab), Si Luo (Oak Ridge National Lab), Zhenghong Bao (Oak Ridge National Lab), Jisue Moon (Oak Ridge National Lab), James Kammert (Oak Ridge National Lab), Xiao Jiang (Oak Ridge National Lab), Weiwei Yang (Oak Ridge National Lab)

Full list of publications (total 191)

1. Zhu, M.; Tian, P.; Cao, X.; Chen, J.; Pu, T.; Shi, B.; Xu, J.; Moon, J.; Wu, Z.; Han, Y.-F., Vacancy engineering of the nickel-based catalysts for enhanced CO2 methanation. *Applied Catalysis B: Environmental* **2021,** *282*, 119561.
2. Zhang, X. Y.; You, R.; Wei, Z. Y.; Jiang, X.; Yang, J. Z.; Pan, Y.; Wu, P. W.; Jia, Q. D.; Bao, Z. H.; Bai, L.; Jin, M. Z.; Sumpter, B.; Fung, V.; Huang, W. X.; Wu, Z. l., Radical Chemistry and Reaction Mechanisms of Propane Oxidative Dehydrogenation over Hexagonal Boron Nitride Catalysts. *Angew Chem Int Edit* **2020,** *59* (21), 8042-8046.
3. Zhang, J. Y.; Zhang, J. B.; Li, M. J.; Wu, Z. L.; Dai, S.; Huang, K., Solvent-free and one-pot synthesis of ultramicroporous carbons with ultrahigh nitrogen contents for sulfur dioxide capture. *Chem Eng J* **2020,** *391*.
4. Yang, J.; Xiao, W.; Chi, X.; Lu, X. X.; Hu, S. Y.; Wu, Z. L.; Tang, W. X.; Ren, Z.; Wang, S. B.; Yu, X. J.; Zhang, L. Z.; Rusydi, A.; Ding, J.; Guo, Y. B.; Gao, P. X., Solar-driven efficient methane catalytic oxidation over epitaxial ZnO/La0.8Sr0.2CoO3 heterojunctions. *Appl Catal B-Environ* **2020,** *265*.
5. Wu, S.; Sun, J.; Li, Q.; Hood, Z. D.; Yang, S.; Su, T.; Peng, R.; Wu, Z.; Sun, W.; Kent, P. R. C.; Jiang, B.; Chisholm, M. F., Effects of Surface Terminations of 2D Bi2WO6 on Photocatalytic Hydrogen Evolution from Water Splitting. *Acs Appl Mater Inter* **2020,** *12* (17), 20067-20074.
6. Wu, P. W.; Tan, S.; Moon, J.; Yan, Z. H.; Fung, V.; Li, N.; Yang, S. Z.; Cheng, Y. Q.; Abney, C. W.; Wu, Z. L.; Savara, A.; Momen, A. M.; Jiang, D. E.; Su, D.; Li, H. M.; Zhu, W. S.; Dai, S.; Zhu, H. Y., Harnessing strong metal-support interactions via a reverse route. *Nat Commun* **2020,** *11* (1).
7. Wang, W. Y.; Hood, Z. D.; Zhang, X. Y.; Ivanov, I. N.; Bao, Z. H.; Su, T. M.; Jin, M. Z.; Bai, L.; Wang, X. W.; Zhang, R. B.; Wu, Z. L., Construction of 2D BiVO4-CdS-Ti3C2Tx Heterostructures for Enhanced Photo-redox Activities. *Chemcatchem* **2020,** *12* (13), 3496-3503.
8. Wang, K.; Fung, V.; Wu, Z. L.; Jiang, D. E., Stable Surface Terminations of a Perovskite Oxyhydride from First-Principles. *J Phys Chem C* **2020,** *124* (34), 18557-18563.
9. Wang, F.; Wu, Z. L., Preface to Special Issue on Advances in Ceria Catalysis. *Chinese J Catal* **2020,** *41* (6), 899-900.
10. Wan, Q.; Fung, V.; Lin, S.; Wu, Z. L.; Jiang, D. E., Perovskite-supported Pt single atoms for methane activation. *J Mater Chem A* **2020,** *8* (8), 4362-4368.
11. Tian, C. C.; Zhang, H. Y.; Zhu, X.; Lin, B.; Liu, X. F.; Chen, H.; Zhang, Y. F.; Mullins, D. R.; Abney, C. W.; Shakouri, M.; Chernikov, R.; Hu, Y. F.; Polo-Garzon, F.; Wu, Z. L.; Fung, V.; Jiang, D. E.; Liu, X. M.; Chi, M. F.; Jimmy, J. L.; Dai, S., A new trick for an old support: Stabilizing gold single atoms on LaFeO3 perovskite. *Appl Catal B-Environ* **2020,** *261*.
12. Shu, Y.; Chen, H.; Chen, N. Q.; Duan, X. L.; Zhang, P. F.; Yang, S. Z.; Bao, Z. H.; Wu, Z. L.; Dai, S., A Principle for Highly Active Metal Oxide Catalysts via NaCl-Based Solid Solution. *Chem* **2020,** *6* (7), 1723-1741.
13. Polo-Garzon, F.; Blum, T. F.; Fung, V.; Bao, Z. H.; Chen, H.; Huang, Z. N.; Mahurin, S. M.; Dai, S.; Chi, M. F.; Wu, Z. L., Alcohol-Induced Low-Temperature Blockage of Supported-Metal Catalysts for Enhanced Catalysis. *Acs Catal* **2020,** *10* (15), 8515-8523.
14. Moon, J.; Cheng, Y. Q.; Daemen, L. L.; Li, M. J.; Polo-Garzon, F.; Ramirez-Cuesta, A. J.; Wu, Z. L., Discriminating the Role of Surface Hydride and Hydroxyl for Acetylene Semihydrogenation over Ceria through In Situ Neutron and Infrared Spectroscopy. *Acs Catal* **2020,** *10* (9), 5278-5287.
15. Li, M. J.; Tian, M. K.; Chen, H.; Mahurin, S. M.; Wu, Z. L.; Dai, S., H2O-prompted CO(2)capture on metal silicatesin situgenerated from SBA-15. *Rsc Advances* **2020,** *10* (48), 28731-28740.
16. Kammert, J.; Moon, J.; Wu, Z. L., A review of the interactions between ceria and H-2 and the applications to selective hydrogenation of alkynes. *Chinese J Catal* **2020,** *41* (6), 901-914.

17. Kammert, J.; Moon, J.; Cheng, Y. Q.; Daemen, L.; Irle, S.; Fung, V.; Liu, J.; Page, K.; Ma, X. H.; Phaneuf, V.; Tong, J. H.; Ramirez-Cuesta, A. J.; Wu, Z. L., Nature of Reactive Hydrogen for Ammonia Synthesis over a Ru/C12A7 Electride Catalyst. *J Am Chem Soc* **2020,** *142* (16), 7655-7667.
18. Ji, Y. Y.; Bai, S. L.; Xu, D. Y.; Qian, D. L.; Wu, Z. L.; Song, Y.; Pace, R.; Crocker, M.; Wilson, K.; Lee, A.; Harris, D.; Scapens, D., Pd-promoted WO3-ZrO2 for low temperature NOx storage. *Appl Catal B-Environ* **2020,** *264*.
19. Huang, R. H.; Fung, V.; Wu, Z. L.; Jiang, D. E., Understanding the conversion of ethanol to propene on In 2 O 3 from first principles. *Catal Today* **2020,** *350*, 19-24.
20. Fung, V.; Hu, G.; Wu, Z.; Jiang, D.-e., Hydrogen in Nanocatalysis. *The Journal of Physical Chemistry Letters* **2020,** *11* (17), 7049-7057.
21. Fung, V.; Hu, G.; Wu, Z.; Jiang, D.-e., Descriptors for Hydrogen Evolution on Single Atom Catalysts in Nitrogen-Doped Graphene. *The Journal of Physical Chemistry C* **2020,** *124* (36), 19571-19578.
22. da Silva, A. G. M.; Fernandes, C. G.; Hood, Z. D.; Peng, R.; Wu, Z. L.; Dourado, A. H. B.; Parreira, L. S.; de Oliveira, D. C.; Camargo, P. H. C.; de Torresi, S. I. C., PdPt-TiO2 nanowires: correlating composition, electronic effects and O-vacancies with activities towards water splitting and oxygen reduction. *Appl Catal B-Environ* **2020,** *277*.
23. Bao, Z. H.; Fung, V.; Polo-Garzon, F.; Hood, Z. D.; Cao, S. H.; Chi, M. F.; Bai, L.; Jiang, D. E.; Wu, Z. L., The interplay between surface facet and reconstruction on isopropanol conversion over SrTiO3 nanocrystals. *J Catal* **2020,** *384*, 49-60.
24. Yusuf, S.; Neal, L.; Bao, Z. H.; Wu, Z. L.; Li, F. X., Effects of Sodium and Tungsten Promoters on Mg6MnO8-Based Core-Shell Redox Catalysts for Chemical Looping-Oxidative Dehydrogenation of Ethane. *Acs Catal* **2019,** *9* (4), 3174-3186.
25. Ye, J. H.; Bai, L.; Liu, B. Y.; Tian, H. J.; Hu, J. L.; Polo-Garzon, F.; Mayes, R. T.; Wu, Z. L.; Fang, Y. X., Fabrication of a Pillared ZSM-5 Framework for Shape Selectivity of Ethane Dehydroaromatization. *Ind Eng Chem Res* **2019,** *58* (17), 7094-7106.
26. Wu, P. W.; Wu, Z. L.; Mullins, D. R.; Yang, S. Z.; Han, X.; Zhang, Y. F.; Foo, G. S.; Li, H. M.; Zhu, W. S.; Dai, S.; Zhu, H. Y., Promoting Pt catalysis for CO oxidation via the Mott-Schottky effect. *Nanoscale* **2019,** *11* (40), 18568-18574.
27. Wang, S. T.; Yu, Y. C.; Luo, S.; Cheng, X. P.; Feng, G. Y.; Zhang, Y. F.; Wu, Z. L.; Compagnini, G.; Pooran, J.; Hu, A. M., All-solid-state supercapacitors from natural lignin-based composite film by laser direct writing. *Appl Phys Lett* **2019,** *115* (8).
28. Su, T. M.; Qin, Z. Z.; Ji, H. B.; Wu, Z. L., An overview of photocatalysis facilitated by 2D heterojunctions. *Nanotechnology* **2019,** *30* (50).
29. Su, T. M.; Hood, Z. D.; Naguib, M.; Bai, L.; Luo, S.; Rouleau, C. M.; Ivanoy, I. N.; Ji, H. B.; Qin, Z. Z.; Wu, Z. L., Monolayer Ti3C2Tx as an Effective Co-catalyst for Enhanced Photocatalytic Hydrogen Production over TiO2. *Acs Appl Energ Mater* **2019,** *2* (7), 4640-4651.
30. Su, T. M.; Hood, Z. D.; Naguib, M.; Bai, L.; Luo, S.; Rouleau, C. M.; Ivanov, I. N.; Ji, H. B.; Qin, Z. Z.; Wu, Z. L., 2D/2D heterojunction of Ti3C2/g-C3N4 nanosheets for enhanced photocatalytic hydrogen evolution. *Nanoscale* **2019,** *11* (17), 8138-8149.
31. Polo-Garzon, F.; Luo, S.; Cheng, Y. Q.; Page, K. L.; Ramirez-Cuesta, A. J.; Britt, P. F.; Wu, Z. L., Neutron Scattering Investigations of Hydride Species in Heterogeneous Catalysis. *Chemsuschem* **2019,** *12* (1), 93-103.
32. Polo-Garzon, F.; Fung, V.; Nguyen, L.; Tang, Y.; Tao, F.; Cheng, Y. Q.; Daemen, L. L.; Ramirez-Cuesta, A. J.; Foo, G. S.; Zhu, M. H.; Wachs, I. E.; Jiang, D. E.; Wu, Z. L., Elucidation of the Reaction Mechanism for High-Temperature Water Gas Shift over an Industrial-Type Copper-Chromium-Iron Oxide Catalyst. *J Am Chem Soc* **2019,** *141* (19), 7990-7999.
33. Polo-Garzon, F.; Bao, Z. H.; Zhang, X. Y.; Huang, W. X.; Wu, Z. L., Surface Reconstructions of Metal Oxides and the Consequences on Catalytic Chemistry. *Acs Catal* **2019,** *9* (6), 5692-5707.
34. Luo, S.; Liu, J.; Wu, Z. L., Interaction of SO2 with ZnO Nanoshapes: Impact of Surface Polarity. *J Phys Chem C* **2019,** *123* (18), 11772-11780.

35. Liu, X. F.; Hood, Z. D.; Zheng, Q.; Jin, T.; Foo, G. S.; Wu, Z. L.; Tian, C. C.; Guo, Y. L.; Dai, S.; Zhan, W. C.; Zhu, H. Y.; Chi, M. F., Optimizing the structural configuration of FePt-FeOx nanoparticles at the atomic scale by tuning the post-synthetic conditions. *Nano Energy* **2019,** *55*, 441-446.
36. Hulsey, M. J.; Zhang, B.; Ma, Z. R.; Asakura, H.; Do, D. A.; Chen, W.; Tanaka, T.; Zhang, P.; Wu, Z. L.; Yan, N., In situ spectroscopy-guided engineering of rhodium single-atom catalysts for CO oxidation. *Nat Commun* **2019,** *10*.
37. Gao, Y. J.; Huang, R. H.; Wang, J. G.; Wu, Z. L.; Jiang, D. E., Effect of Hydrogen-Induced Metallization on Chemisorption. *J Phys Chem C* **2019,** *123* (24), 15171-15175.
38. Bai, L.; Polo-Garzon, F.; Bao, Z. H.; Luo, S.; Moskowitz, B. M.; Tian, H. J.; Wu, Z. L., Impact of Surface Composition of SrTiO3 Catalysts for Oxidative Coupling of Methane. *Chemcatchem* **2019,** *11* (8), 2107-2117.
39. Zhu, M. H.; Li, B.; Jehng, J. M.; Sharma, L.; Taborda, J.; Zhang, L. H.; Stach, E.; Wachs, I. E.; Wu, Z. L.; Baltrusaitis, J., Molecular structure and sour gas surface chemistry of supported K2O/WO3/Al2O3 catalysts. *Appl Catal B-Environ* **2018,** *232*, 146-154.
40. Zhang, S. R.; Tang, Y.; Nguyen, L.; Zhao, Y. F.; Wu, Z. L.; Goh, T. W.; Liu, J. J. Y.; Li, Y. Y.; Zhu, T.; Huang, W. Y.; Frenkel, A. I.; Li, J.; Tao, F. F., Catalysis on Singly Dispersed Rh Atoms Anchored on an Inert Support. *Acs Catal* **2018,** *8* (1), 110-121.
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42. Su, T. M.; Shao, Q.; Qin, Z. Z.; Guo, Z. H.; Wu, Z. L., Role of Interfaces in Two-Dimensional Photocatalyst for Water Splitting. *Acs Catal* **2018,** *8* (3), 2253-2276.
43. Su, T. M.; Peng, R.; Hood, Z. D.; Naguib, M.; Ivanov, I. N.; Keum, J. K.; Qin, Z. Z.; Guo, Z. H.; Wu, Z. L., One-Step Synthesis of Nb2O5/C/Nb2C (MXene) Composites and Their Use as Photocatalysts for Hydrogen Evolution. *Chemsuschem* **2018,** *11* (4), 688-699.
44. Song, Y.; Johnson, D.; Peng, R.; Hensley, D. K.; Bonnesen, P. V.; Liang, L. B.; Huang, J. S.; Yang, F. C.; Zhang, F.; Qiao, R.; Baddorf, A. P.; Tschaplinski, T. J.; Engle, N. L.; Hatzell, M. C.; Wu, Z. L.; Cullen, D. A.; Meyer, H. M.; Sumpter, B. G.; Rondinone, A. J., A physical catalyst for the electrolysis of nitrogen to ammonia. *Sci Adv* **2018,** *4* (4).
45. Polo-Garzon, F.; Wu, Z. L., Acid-base catalysis over perovskites: a review. *J Mater Chem A* **2018,** *6* (7), 2877-2894.
46. Polo-Garzon, F.; Fung, V.; Liu, X. M.; Hood, Z. D.; Bickel, E. E.; Bai, L.; Tian, H. J.; Foo, G. S.; Chi, M. F.; Jiang, D. E.; Wu, Z. L., Understanding the Impact of Surface Reconstruction of Perovskite Catalysts on CH4 Activation and Combustion. *Acs Catal* **2018,** *8* (11), 10306-10315.
47. Peng, R.; Wu, Z. L., Role of Interfaces at Nano-Architectured Photocatalysts for Hydrogen Production from Water Splitting. In *Multifunctional Nanocomposites for Energy and Environmental Applications*, Guo, Z.; Chen, Y.; Lu, N. L., Eds. 2018; pp 403-438.
48. Luo, Y. C.; Fan, S. Y.; Yu, W. Q.; Wu, Z. L.; Cullen, D. A.; Liang, C. L.; Shi, J. Y.; Su, C. Y., Fabrication of Au-25(SG)(18)-ZIF-8 Nanocomposites: A Facile Strategy to Position Au-25(SG)(18) Nanoclusters Inside and Outside ZIF-8. *Adv Mater* **2018,** *30* (6).
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52. Huang, W. X.; Wu, Z. L.; Tang, J. W.; Wei, W. D.; Guo, X. F., Surface chemistry connecting heterogeneous catalysis, photocatalysis and plasmonic catalysis. *Chinese Chem Lett* **2018,** *29* (6), 725-726.

53. Huang, R. H.; Fung, V.; Zhang, Y. F.; Mullins, D. R.; Wu, Z. L.; Jiang, D. E., Understanding Methanol Coupling on SrTiO3 from First Principles. *J Phys Chem C* **2018,** *122* (13), 7210-7216.
54. Hu, G. X.; Wu, Z. L.; Jiang, D. E., Stronger-than-Pt hydrogen adsorption in a Au-22 nanocluster for the hydrogen evolution reaction. *J Mater Chem A* **2018,** *6* (17), 7532-7537.
55. Hu, G. X.; Wu, Z. L.; Jiang, D. E., First Principles Insight into H-2 Activation and Hydride Species on TiO2 Surfaces. *J Phys Chem C* **2018,** *122* (35), 20323-20328.
56. Hu, G. X.; Wu, Z. L.; Dai, S.; Jiang, D. E., Interface Engineering of Earth-Abundant Transition Metals Using Boron Nitride for Selective Electroreduction of CO2. *Acs Appl Mater Inter* **2018,** *10* (7), 6694-6700.
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58. Fung, V.; Polo-Garzon, F.; Wu, Z. L.; Jiang, D. E., Exploring perovskites for methane activation from first principles. *Catal Sci Technol* **2018,** *8* (3), 702-709.
59. Foo, G. S.; Hood, Z. D.; Wu, Z. L., Shape Effect Undermined by Surface Reconstruction: Ethanol Dehydrogenation over Shape-Controlled SrTiO3 Nanocrystals. *Acs Catal* **2018,** *8* (1), 555-565.
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