Final Technical Report

A. SCIENTIFIC/TECHNICAL REPORTS

Content. The final scientific/technical report must include the following information and any other information identified under Special Instructions on the Federal Assistance Reporting Checklist:

1. **DOE Award No:** DE-SC0001058
   Recipient: Louisiana State University
   Project Title: Center for Atomic-Level Catalyst Design
   Project Director: James J. Spivey
   Consortium/Teaming Members:

   - Louisiana State University – Challa Kumar, E Ward Plummer, Richard Kurtz, Phillip Sprunger, Kerry Dooley, John Flake, Gregory Griffin, Amitava Roy, Bill Shelton, Louis Haber, Ken Lopata
   - Louisiana Tech University/ Grambling University– Tabbetha Dobbins
   - Grambling University – Naidu Seetala
   - Clemson University – David Bruce, J. Goodwin
   - University of Florida – Susan Sinnott
   - Ohio State University - Aravind Asthagiri
   - Georgia Tech Research Corp – David Sholl
   - Pennsylvania State University – Michael Janik
   - Texas A&M Research Foundation – D. Wayne Goodman, Li Liu
   - Utrecht University - Krijin de Jong, Petra de Jongh, Harry Bitter
   - Vienna University of Technology – Ulrike Diebold
   - Oak Ridge National Lab – Ye Xu

2. **Authorized distribution limitation notices:** None

3. **Provide an executive summary**

   The research summarized here has the goal of developing a fundamental understanding of how catalysts work. These materials are demonstrably essential to our daily life, from the cars we drive to the clothes we wear. Our Center advances the science behind how we prepare, analyze, and describe catalysts. This has been identified by one of the documents guiding Federal research objectives (*Directing Matter and Energy: Five Challenges for Science and the Imagination*): *"Major challenges in heterogeneous catalysis are to more clearly define the nature of the active sites, to engineer at the molecular level catalysis with designed properties in three dimensions, and to create new catalysts for new transformations."* This directly addresses this objective.

4. Provide a comparison of the actual accomplishments with the goals and objectives of the project.

Goals and objectives	Actual accomplishments (examples)
Advance the capabilities of computational catalysis	• Characterize electrochemical reduction of CO_2 including kinetics and aqueous environment at Cu and Fe electrodes. • Evaluate reaction behavior of CO_2 and key intermediates at Cu electrodes.
Advance the capabilities of catalyst characterization	• Characterize the behavior of nanoparticles deposited on conductive oxides and in an anode matrix. • Determine similarities and differences of the effects of transition metal dopants.
Advance the capabilities of catalyst synthesis	• Synthesize REO/TMO catalysts capable of reforming/ cracking naphthalene. • Determine the vacancy formation energies associated with Mn-doping.

5. Summarize project activities for the entire period of funding

The original hypothesis leading to the Center is that the disciplines of catalysis synthesis, characterization, and computation can significantly be advanced by developing a Center in which the synergism in these three skills can be enhanced. The impact of their activities can be clear, e.g, in their research products as documented in journal papers. Of the all peer-reviewed publications produced in our current Center, more than half include co-authors more than one institution.

The activities in the entire period of funding have been described in detail in an invited, peer-reviewed scientific journal paper: (Spivey et al., ,dx.doi.org/10.1021/jp502556u | J. Phys. Chem. C 2014, 118, 20043−20069). This includes 17 co-authors.

6. Identify products developed under the award and technology transfer activities, such as:

a. Publications

1. Kamal Choudhary, Tao Liang, Kiran Mathew, Benjamin Revard, Aleksandr Chernatynskiy, Simon R. Phillpot, Richard G. Hennig, Susan B. Sinnott, Dynamical

properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials, Computational Materials Science, Volume 113, 15 February 2016, Pages 80-87, ISSN 0927-0256,

2. Felipe Polo-Garzon, Ming He, David A. Bruce, Ab initio derived reaction mechanism for the dry reforming of methane on Rh doped pyrochlore catalysts, Journal of Catalysis, Volume 333, January 2016, Pages 59-70, ISSN 0021-9517
3. Chelliah V. Navin, Katla Sai Krishna, G. Lisa Bovenkamp-Langlois, Jeffery T. Miller, Soma Chattopadhyay, Tomohiro Shibata, Yaroslav Losovyj, Varshni Singh, Chandra Theegala, Challa S.S.R. Kumar, Investigation of the synthesis and characterization of platinum-DMSA nanoparticles using millifluidic chip reactor, Chemical Engineering Journal, Volume 281, 1 December 2015, Pages 81-86, ISSN 1385-8947
4. William C. McKee, Vincent Meunier, Ye Xu, Reconciling the electronic and geometric corrugations of the hexagonal boron nitride and graphene nanomeshes, Surface Science, Volume 642, December 2015, Pages L16-L19, ISSN 0039-6028
5. Zi Wang, James J. Spivey, Effect of ZrO2, Al2O3 and La2O3 on cobalt–copper catalysts for higher alcohols synthesis, Applied Catalysis A: General, Volume 507, 25 October 2015, Pages 75-81, ISSN 0926-860X
6. Matthew D. Krcha, Kerry M. Dooley, Michael J. Janik, Alkane reforming on partially sulfided CeO2 (1 1 1) surfaces, Journal of Catalysis, Volume 330, October 2015, Pages 167-176, ISSN 0021-9517
7. Matthew D. Krcha, Michael J. Janik, Catalytic propane reforming mechanism over Mn-Doped CeO2 (111), Surface Science, Volume 640, October 2015, Pages 119-126, ISSN 0039-6028
8. Nitin Kumar, Maryam Shojaee, JJ Spivey, Catalytic bi-reforming of methane: from greenhouse gases to syngas, Current Opinion in Chemical Engineering, Volume 9, August 2015, Pages 8-15, ISSN 2211-3398
9. Prieto, G., Beijer, S., Smith, M. L., He, M., Au, Y., Wang, Z., Bruce, D. A., de Jong, K. P., Spivey, J. J. and de Jongh, P. E. (2014), Design and Synthesis of Copper–Cobalt Catalysts for the Selective Conversion of Synthesis Gas to Ethanol and Higher Alcohols. Angew. Chem., 126: 6515–6519. doi:10.1002/ange.201402680
10. Yue Y, Xu Y and Liu L. Two-Dimensional Gold Islands on Graphene/Ru (0001) Moiré Structure. Ann J Materials Sci Eng. 2014;1(1): 2.Dieh Teng, Lasse B. Vilhelmsen, David S. Sholl, Investigating energetics of Au8 on graphene/Ru(0001) using a genetic algorithm and density functional theory, Surface Science, Volume 628, October 2014, Pages 98-103, ISSN 0039-6028

11. Mark J. Noordhoek, Tao Liang, Tsu-Wu Chiang, Susan B. Sinnott, Simon R. Phillpot, Mechanisms of Zr surface corrosion determined via molecular dynamics simulations with charge-optimized many-body (COMB) potentials, Journal of Nuclear Materials, Volume 452, Issues 1–3, September 2014, Pages 285-295, ISSN 0022-3115
12. Dieh Teng, David S. Sholl, Adsorption and diffusion of Rh and Au dimers and trimers on graphene/Ru(0001), Surface Science, Volume 626, August 2014, Pages 6-13, ISSN 0039-6028
13. Tao Liang, Yu-Ting Cheng, Xiaowa Nie, Wenjia Luo, Aravind Asthagiri, Michael J. Janik, Evan Andrews, John Flake, Susan B. Sinnott, Molecular dynamics simulations of CO2 reduction on Cu(111) and Cu/ZnO(10 0) using charge optimized many body potentials, Catalysis Communications, Volume 52, 5 July 2014, Pages 84-87, ISSN 1566-7367
14. Xiaowa Nie, Gregory L. Griffin, Michael J. Janik, Aravind Asthagiri, Surface phases of Cu2O(111) under CO2 electrochemical reduction conditions, Catalysis Communications, Volume 52, 5 July 2014, Pages 88-91, ISSN 1566-7367
15. Devendra Pakhare, Viviane Schwartz, Victor Abdelsayed, Daniel Haynes, Dushyant Shekhawat, James Poston, James Spivey, Kinetic and mechanistic study of dry (CO2) reforming of methane over Rh-substituted La2Zr2O7 pyrochlores, Journal of Catalysis, Volume 316, July 2014, Pages 78-92, ISSN 0021-9517
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17. Krishna, K. S., Tarakeshwar, P., Mujica, V. and Kumar, C. S. S. R. (2014), Chemically Induced Magnetism in Atomically Precise Gold Clusters. Small, 10: 907–911. doi:10.1002/smll.201302393
18. Xiaowa Nie, Wenjia Luo, Michael J. Janik, Aravind Asthagiri, Reaction mechanisms of CO2 electrochemical reduction on Cu(1 1 1) determined with density functional theory, Journal of Catalysis, Volume 312, April 2014, Pages 108-122, ISSN 0021-9517
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21. Jackelyn A. Martinez, Dundar E. Yilmaz, Tao Liang, Susan B. Sinnott, Simon R. Phillpot, Fitting empirical potentials: Challenges and methodologies, Current Opinion in Solid

State and Materials Science, Volume 17, Issue 6, December 2013, Pages 263-270, ISSN 1359-028

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23. Tao Liang, Tzu-Ray Shan, Yu-Ting Cheng, Bryce D. Devine, Mark Noordhoek, Yangzhong Li, Zhize Lu, Simon R. Phillpot, Susan B. Sinnott, Classical atomistic simulations of surfaces and heterogeneous interfaces with the charge-optimized many body (COMB) potentials, Materials Science and Engineering: R: Reports, Volume 74, Issue 9, September 2013, Pages 255-279, ISSN 0927-796X
24. Gonzalo Prieto, Johannes D. Meeldijk, Krijn P. de Jong, Petra E. de Jongh, Interplay between pore size and nanoparticle spatial distribution: Consequences for the stability of CuZn/SiO2 methanol synthesis catalysts, Journal of Catalysis, Volume 303, July 2013, Pages 31-40, ISSN 0021-9517
25. Sarthak Gaur, Hongyi Wu, George G. Stanley, Karren More, Challa S.S.R. Kumar, James J. Spivey, CO oxidation studies over cluster-derived Au/TiO2 and AUROlite™ Au/TiO2 catalysts using DRIFTS, Catalysis Today, Volume 208, 1 June 2013, Pages 72-81, ISSN 0920-5861
26. Devendra Pakhare, Christopher Shaw, Daniel Haynes, Dushyant Shekhawat, James Spivey, Effect of reaction temperature on activity of Pt- and Ru-substituted lanthanum zirconate pyrochlores (La2Zr2O7) for dry (CO2) reforming of methane (DRM), Journal of CO2 Utilization, Volume 1, June 2013, Pages 37-42, ISSN 2212-9820
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b. Web site or other Internet sites that reflect the results of this project;

www.efrc.lsu.edu

https://sites01.lsu.edu/wp/lsuresearch/2015/01/24/power-center-lsu-on-clean-energy/

c. Networks or collaborations fostered

Collaborations have been fostered among the 11 partner institutions:

Louisiana State University
Pennsylvania State University
University of Florida
Georgia Institute of Technology
Institute of Applied Physics, Vienna, Austria
Clemson University
Utrecht University, Utrecht, Netherlands
Grambling University
Texas A&M
Oak Ridge National Lab
Ohio State University

d. Technologies/Techniques

Technologies and techniques have been developed in each project. These are described in detail in the following paper: Spivey et al., ,dx.doi.org/10.1021/jp502556u | J. Phys. Chem. C 2014, 118, 20043−20069.

e. Inventions/Patent Applications, licensing agreements

In 2012, a technology disclosure (internal LSU document): , "Millifluidic Catalyst Test platform." , was reported. The start-up company, Millifluidica LLC

(www.millifluidica.com) was formed based on this EFRC research.

f. Other products

No additional products**.**

7. For projects involving computer modeling, provide the following information with the final report:

No additional models other than those described in the above paper: Spivey et al., ,dx.doi.org/10.1021/jp502556u | J. Phys. Chem. C 2014, 118, 20043−20069.