DATA SCIENCE:
Opportunities to Transform Chemical Sciences and Engineering
A Chemical Sciences Roundtable Workshop

DAY 1
Date – February 27, 2018
Location – NAS Building, Room 125

8:30 AM  Opening Remarks
Bruce Garrett, CSR Planning Committee Member
Division Director, Chemical Sciences, Geosciences and Biosciences
US Department of Energy

8:40 AM  What is Data Science?
Andrew Ferguson
Assistant Professor of Materials Science and Engineering
University of Illinois at Urbana-Champaign

9:20 AM  What Can Data Science Do for Me?
Patrick Riley
Principal Engineer
Google

10:00 AM  Data Science in Industry
Salvador Garcia-Munoz
Senior Engineering Advisor
Eli Lilly and Company

10:40 AM  Break

11:00 AM  Untapped Data Resources
Thomas Bligaard
Deputy Director, Senior Staff Scientist
SUNCAT Center for Interface Science and Catalysis
SLAC National Accelerator Laboratory
11:40 AM  Panel Discussion (Moderator, Bruce Garrett; Panelists, Morning Speakers): How can data science be used to gain insights or new knowledge from data resources? What are the barriers that are preventing broader adoption of data sciences in the chemical sciences and engineering

12:30 PM  LUNCH BREAK

1:30 PM  Creating Data Science Programs in Academia
  
  Thomas Ewing  
  Associate Dean of Graduate Studies and Research  
  Virginia Tech

2:15 PM  ADJOURN TO BREAKOUT SESSIONS

Breakout 1: Data Analytics  
Co-chairs:  Sharon Glotzer  
Department Chair and Distinguished Professor  
Department of Chemical Engineering  
University of Michigan  
Bryce Meredig  
Cofounder and Chief Science Officer  
Citrine Informatics

Breakout 2: Data Quality Assessment  
Co-chairs:  David Higdon  
Professor, Social Decision Analytics Laboratory  
Biocomplexity Institute of Virginia Tech  
Carlos Gonzalez, CSR Planning Committee Member  
Division Chief, Chemical Sciences Division  
National Institutes of Standards and Technology

Breakout 3: Data Management and Translation  
Co-chairs:  Jens Hummelshøj  
Materials Design & Discovery Program Manager  
Toyota Research Institute  
John Gregoire, CSR Planning Committee Member  
Thrust Coordinator for Photoelectrocatalysis  
DOE Joint Center for Artificial Photosynthesis  
Caltech University  
Assoc. Director, NSF Computational Sustainability Network
DAY 2
Date – February 28, 2018
Location – NAS Building, Room 125

8:30 AM   Reporting from Breakout Groups

10:00 AM   Panel Discussion: Training a Future Generation of Chemists/Chemical Engineers

Moderator:   Leo Chiang, CSR Planning Committee Member
             Associate Technology Director
             The Dow Chemical Company

Panelists:   Richard Braatz
             Edwin R. Gilliland Professor
             Massachusetts Institute of Technology

            Lloyd Colegrove
             Data Services Director
             The Dow Chemical Company

            Melissa Cragin
             Executive Director, Midwest Big Data Hub
             University of Illinois at Urbana-Champaign

            Al Hero
             John H. Holland Distinguished University Professor
             Jamison and Betty Williams Professor of Engineering
             University of Michigan

            Rebecca Nugent
             Professor, Department of Statistics
             Carnegie Mellon University
11:30 AM    Closing Remarks
            Bruce Garrett, CSR Planning Committee Member
            Division Director, Chemical Sciences, Geosciences and Biosciences
            US Department of Energy

12:00 PM    Workshop Concludes