FUEL

DIVISION OF FUEL CHEMISTRY

C. Liu and V. Subramani, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:
Advances in Biofuels and Bioproducts: Life Cycle Analysis and Sustainability (see *AGRO*, Mon)
Nanoscience: Fuel Cells and Energy Storage (see *INOR*, Mon)
Green Chemistry for a Sustainable World (see *I&EC*, Tue)
Energy Sustainability of the Water Infrastructure Using Microbial Fuel Cell Based Technologies (see *ENVR*, Wed - Thu)
Biocatalysis for Biofuels and Bioproducts (see *AGFD*, Tue - Wed)
SOCIAL EVENTS:
Dinner, 6:00 PM: Tue
Program Planning Meeting, 1:00 PM: Sun
BUSINESS MEETING:
Executive Council Meeting, 3:00 PM: Sun
Business Meeting, 12:00 PM: Mon

SUNDAY MORNING

Section A

InterContinental San Francisco
Grand Ballroom A

Green Chemistry on Fuels of the Future

Analytic and Characterization

M. Dong, R. Glaeser, W.-L. Jang, and C. Liu, *Organizers*
F. Besenbacher, and L. Wan, *Presiding*

8:25 Opening Remarks.

8:30 1. Impacts of biodiesel and Fischer-Tropsch fuels on the reactivity and nanostructure of diesel soot. **K. Yehliu**, R. L. Vander Wal, A. L. Boehman

8:50 2. Analysis of solvent dyes in refined petroleum products by electrospray ionization/mass spectrometry. **C. E. Rostad**

9:10 3. Raman spectroscopy for the study of soot crystalline structure and soot oxidative reactivity. **H. J. Seong**, **A. L. Boehman**

9:30 4. Applications of ion chromatography for the analysis of fuels and biofuels: Green chemistry approach. **J. C. Gandhi**

9:50 Intermission.

10:00 5. Electrochemistry of nanostructured electrode materials in Li-ion battery and DMFC. **L.-J. Wan**

10:45 6. Catalytic model systems studied by high-resolution, video-rate scanning tunneling microscopy. **F. Besenbacher**

11:30 7. Comparative exergy analysis of NREL thermochemical biomass-to-ethanol conversion process designs. **K.-Y. Teh**, A. E. Lutz, C. R. Shaddix, A. Dutta, M. Biddy, A. Aden

11:50 8. Single-cell diesel mining: Direct and quantitative monitoring of microalgal oil production in vivo by laser-trapping Raman spectroscopy. **H. Wu**, J. V. Volponi, S. Singh

Section B

InterContinental San Francisco
InterContinental Ballroom B

Separation and Catalysis Needs for Renewable Energy

Separation

Cosponsored by CATL (probationary)
G. Lu, *Presiding*
S. Dai, *Organizer, Presiding*

8:20 9. Sol-gel derived organic-inorganic silica membranes with controlled silica network size. **M. Kanezashi**, K. Yada, T. Yoshioka, T. Tsuru

8:40 10. Separation of hydrocarbons from sand using ionic liquids. **P. C. Painter**, P. Williams, E. Mannebach

9:00 11. Purification effects on the gas sorption in single walled carbon nanotubes. **A. Surapathi**, E. Marand

9:20 12. On the development of alkaline membrane fuel cells. **L. Zhuang**

9:50 13. Measurement and modeling of liquid-liquid phase equilibria for removal of alcohols from water with ionic liquids. A. Chapeaux, L. D. Simoni, T. S. Ronan, M. A. Stadtherr, **J. F. Brennecke**

10:20 Intermission.

10:30 14. Wood delignification using polyoxometalates in ionic liquid. N. Sun, X. Jiang, M. L. Maxim, **R. D. Rogers**

11:00 15. Membranes for aggressive CO_2 separation applications. **W. J. Koros**

11:30 16. Simplified method to extract biofuels from aqueous mixtures using organophilic silicas that rapidly and reversibly swell. **P. L. Edmiston**

11:50 17. Novel ionic liquids for membrane-based separation of carbon dioxide. **S. M. Mahurin**, J. Lee, G. Baker, S. Dai

12:10 18. Driving forces for adsorption of polyols onto zeolites from aqueous solutions. **E. Mallon**, A. Bhan, M. Tsapatsis

InterContinental San Francisco
Howard

Fuel Chemistry and Electrochemistry for Fuel Cells

Electrocatalysis

Cosponsored by CATL (probationary) and PHYS
R. Kostecki, and S. Sui, *Organizers*
E. J. Cairns, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 19. Selective oxidation of CO on Au-TiO_2 catalysts on a structured carbon support. N. Hammer, T. Zscherpe, D. Chen, **M. Ronning**

8:50 20. New mechanism for carbon monoxide adsorption on platinum and platinum-ruthenium surfaces of direct methanol fuel cells. **N. Dimakis**, T. Mion, E. S. Smotkin

9:10 21. Effect of particle size and support on the catalytic activity of Platinum nanoparticles for oxygen reduction reaction. **V. Viswanathan**, F. Y.-F. Wang, H. Pitsch

9:30 22. $Pt_{1-x}Ru_x$ sputtered thin films for DMFC catalyst applications. **A. Dameron**, J. Leisch, K. O'Neill, S. Studer, H. Dinh, R. O'Hayre, T. Gennett

9:50 23. Electrocatalysis of ethanol oxidation on doped octahedral molecular sieves of manganese. **G. V. Sokolsky**, **S. V. Ivanov**, T. F. Lobunets, M. V. Demchenko, N. D. Ivanova, T. V. Tomila, O. V. Kobylinskaya

10:10 24. Designed synthesis of WC/crystalline nanocarbon composites and their application exploration in DMFC. **H. Fu**

10:30 Intermission.

Section C

InterContinental San Francisco
Howard

Fuel Chemistry and Electrochemistry for Fuel Cells

Membranes

E. J. Cairns, and R. Kostecki, *Organizers*
S. Sui, *Organizer, Presiding*

10:40 25. Self-organized hybrid proton exchange membranes, exhibiting high ionic conductivity. **M. Barboiu**, M. Michau

11:00 26. Investigation of PBI high-temperature membranes for direct methanol fuel cells. **E. B. Fox**, B. L.

Garcia-Diaz, H. R. Colon-Mercado, K. Herrington

11:20 27. Immobilization of composite inorganic additive on PFSA ionomers for improved performance. **R. Janarthanan**, A. M. Herring, G. M. Haugen, S. J. Hamrock

11:40 28. Toward high temperature Pemfc membranes based on Pcils hosted by functional polymers. **J.-Y. Sanchez**, C. Iojoiu, J.-C. Leprêtre, M. Martinez, M. Hanna, L. Cointeaux, Y. Molmeret, N. El Kissi, P. Judeinstein, D. Langevin, R. Mercier

12:00 29. Viscoelastic and transport properties of hydrophilic-hydrophobic multiblock copolymers. **Y. Fan**, C. J. Cornelius, J. McGrath, H.-S. Lee, Y. Chen

12:20 30. Thermal behavior and conductivity of rubidium dihydrogen phosphate (RbH_2PO_4) at high temperature. **Z. Li**, T. Tang

Section D

InterContinental San Francisco
Union Square

CO_2 Capture, Conversion and Utilization

Catalytic and Electrochemical Conversion of CO_2

V. S.-Y. Lin, and B.-L. Su, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 31. Nanostructured materials for green chemistry. **J. Y. Ying**

9:05 32. Progresses in carbonate looping process: Materials and applications. L. He, T. Zhao, S. K. Sultana, M. Rønnring, **D. Chen**

9:30 33. Selective production of solid ammonium bicarbonate and ammonium carbamate in the process of carbon dioxide capture by ammonia solutions: A feasible process to produce urea in mild conditions. **F. Mani**, F. Barzagli, M. Peruzzini

9:50 34. Oxidative dehydrogenation of ethane with CO2 over nanocrystallite MgAl2O4 supported cobalt-based catalysts. **X. Zhang**

10:10 Intermission.

10:20 35. CO_2 conversion to fuels: Prospects and opportunities. **G. Centi**, S. Perathoner

10:55 36. Laser assisted conversion of carbon dioxide and methane. **J. Kotze**, C. A. Strydom, A. Du Plessis

11:15 37. Dry reforming of methane over a Ni-CaO-ZrO_2 catalyst: Effect of pore structure. N. Sun, F. Xiao, **W. Wei**, **Y. Sun**

11:35 38. Carbon dioxide reforming of methane in stable spark-discharge plasma. X.-S. Li, B. Zhu, **A. Zhu**

Section E

InterContinental San Francisco
Grand Ballroom B

Solar Cells and Solar Fuels

Nanomaterials

H. Jia, Y. Lu, L. Sun, and D. Wang, *Organizers, Presiding*

8:30 39. Photonic fuels and photovoltaics: Application of self-assembled 1D TiO_2 nanotube/wire arrays. **C. A. Grimes**, O. K. Varghese, G. K. Mor, M. Paulose, X. Feng

9:00 40. Semiconductor nanowires for energy conversion. **P. Yang**

9:30 41. Light energy conversion based on quantum dot-sensitized and N-doped metal oxide nanostructures. **J. Z. Zhang**, A. Wolcott, J. Hensel, R. Fitzmorris, Y. Li, X. Yang, G. Wang, W. Smith, Y. Zhao, J. Li, L. Liu, Y. Li

10:00 42. Rational design of photoelectric nanodevices as highly efficient photocatalysts. Y. Qu, **X. Duan**

10:30 43. Photocatalytic reduction of carbon dioxide to fuel using hydrothermally synthesized titania nanotubes **B. Vijayan**, D. Finkelstein Shapiro, P. A. DeSario, N. Dimitrijevic, K. A. Gray

Section E

InterContinental San Francisco
Grand Ballroom B

Solar Cells and Solar Fuels

Cutting Edge Biotech

H. Jia, Y. Lu, L. Sun and D. Wang, *Organizers, Presiding*

11:00 44. Powering the planet with solar fuel. **B. D. Stubbert**, **S. Dasgupta**, **H. B. Gray**

11:45 45. High intensity enzymatic biocatalysis for direct conversion of solar energy into chemicals and fuels. X. Lu, X. Zhao, **P. Wang**

12:15 46. RNA mediated assembly of nanoparticles and the potential for water splitting catalysis. J. L. Rouge, **B. E. Eaton**

12:45 47. Development of a biohybrid micellar system for solar hydrogen production. **H. O'Neill**, X. Liu, E. Lauer, X. Yu, K. Hong

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Robert J. Madix

From Surface Science to Heterogeneous Catalysis: Fundamental Concepts in Surface Reactivity and Catalysis

Sponsored by CATL (probationary), Cosponsored by COLL, FUEL and PETR

Catalysis for Sustainability

CO_2 Conversion and Utilization

Sponsored by CATL (probationary), Cosponsored by FUEL and PETR

Catalysis for Sustainability

Photocatalysis for Fuel Synthesis: Oxide Materials

Sponsored by CATL (probationary), Cosponsored by FUEL

SUNDAY AFTERNOON

Section A

InterContinental San Francisco
Grand Ballroom A

Green Chemistry on Fuels of the Future

Ultraclean Fuels

M. Dong, W.-L. Jang, and C. Liu, *Organizers*
R. Glaeser, *Organizer, Presiding*

1:10 48. H_2 fuel production: Au-based nanocatalysts for methanol steam reforming and the water gas shift reaction. N. Yi, R. Si, H. Saltsburg, **M. Flytzani-Stephanopoulos**

1:55 49. Preventing mercury re-emissions in wet flue gas desulfurization scrubbers at coal-fired power plants using MerControl® 8034 additive. **R. L. Stiles**, P. J. Zinn, J. V. Lu, J. J. Michels, A. M. Leigh, B. A. Keiser

2:15 50. 2,5-Dimethylfuran: Exploring the combustion chemistry of a next-generation biofuel. **W. K. Metcalfe**, J. M. Simmie, H. J. Curran

2:35 51. Ultraclean fuels obtained by hydrodeoxygenation of renewable feedstocks: Deactivation of deoxygenation catalysts. **D. Kubicka**, F. Homola, J. Horácek

Section A

InterContinental San Francisco
Grand Ballroom A

Fuel Chemistry and Electrochemistry for Fuel Cells

Fuel Cell General

E. J. Cairns, and S. Sui, *Organizers*
Y. Li, *Presiding*
R. Kostecki, *Organizer, Presiding*

3:50 52. Pt and/or Pd supported/incorporated catalyst on perovskite-type oxide for water gas shift reaction. **R. Watanabe**, Y. Sekine, H. Takamatsu, Y. Sakamoto, M. Matsukata, E. Kikuchi

4:10 53. Oxidative desulfurization of middle distillate fuels for fuel cell applications. **L. A. Gonzalez**, R. C. Miake-Lye, M. T. Timko, P. Kracke, S. Zhou, J. W. Tester, W. H. Green

4:30 54. Mechanism and performance of an inexpensive monosaccharide biofuel cell. **L. Chetty**, J.-S. Kim, N. H. Zhao, D. Scott, B. Y. Liaw

4:50 55. Hydrogen production by steam reforming of ethanol over supported iron-cobalt catalyst. **Y. Izutsu**, Y. Sekine, A. Kazama, M. Matsukata, E. Kikuchi

5:10 56. Initial research on the activation process for a PEMFC: Phenomenon analysis. **M. Hu**

Section B

InterContinental San Francisco
InterContinental Ballroom B

Separation and Catalysis Needs for Renewable Energy

Catalysis

B.-Q. Xu, *Presiding*
S. Dai, *Organizer, Presiding*

1:00 57. Kinetics and elementary steps of the reverse water-gas shift reaction over Pt catalysts. **C. T. Campbell**, L. G. Cameron, M. Mavrikakis, L. C. Grabow

1:30 58. Pyrolysis behavior of lignin model compounds. **A. C. Buchanan III**, M. K. Kidder, A. Beste

2:00 59. Performance of several nano-ruthenium based catalysts on water gas shift reaction. **Y. Li**, **Z. Mei**, M. Fan

2:20 60. Understanding Hg reactivity on a selective catalytic reduction (SCR) catalyst: V_2O_5. **A. Suarez Negreira**, J. Wilcox

2:40 61. Functionalised polysaccharide derived porous materials for the production of second generation biofuels from waste oils. **R. Luque**, J. M. Campelo, J. H. Clark, J. M. Marinas, A. A. Romero

3:00 62. Role of cobalt oxide on deleterious chlorine ion over PdO/SiO2 for CO oxidation. F. Wang, **G. Lu**

3:20 Intermission.

3:30 63. Pt saving electrocatalysts by the use of colloidal Au and Ag particles. **B.-Q. Xu**, G.-R. Zhang, D. Zhao

4:00 64. Synthesis and fundamental understaning of catalytic materials for sustainable energy. **Y. Wang**

4:30 65. Catalytic dehydrogenation of ethane assisted by hydrogen perselective membrane. **L. Nossova**, T. Giddings, J. Galuszka

4:50 66. Toluene steam reforming over transition metals –doped CeO_2-ZrO_2 suppoted nickel catalysts. **V. Meeyoo**, A. Bampenrat, P. Rangsanvigit, T. Rirksomboon, B. Kitiyanan, J. Schwank

5:10 67. CO_x free hydrogen production from cellulose and calcium hydroxide mixture. **M. Matsumoto**, Y. Kawai, S.-I. Towata, Y. Fukushima, Q. Zhang, F. Saito

5:30 68. Intermolecular C-H bond activation of benzene by a vanadium(III) alkylidene including the stepwise conversion to benzyne. **J. G. Andino Martinez**

Section C

InterContinental San Francisco
Howard

Fuel Chemistry and Electrochemistry for Fuel Cells

Fuel Cell Operations

E. J. Cairns, and S. Sui, *Organizers*
R. Kostecki, *Organizer, Presiding*

1:40 69. Research and development activities of PEMFC durability at DICP. **Z.-G. Shao**, H. Yu, M. Hou, X. Li, L. Zhou, B. Yi

2:00 70. Effects of anode diffusion on direct methanol fuel cell (DMFC) performance. **S. Sui**, **E. Cairns**

2:20 71. Electricity from coal using CO_2 gasifier integrated SOFC system. **C. Q. Fan**, R. J. Stanis, E. Ong

2:40 72. New results on a direct carbon fuel cell based on a composite electrolyte. L. Jia, Q. Liu, C. Xia, J. Yu, **Y. Li**

3:00 73. Chemical and electrochemical performance of solid oxide fuel cells operating on solid carbon. **Z. Shao**, Y. Wu, C. Su

Section D

InterContinental San Francisco
Union Square

Correlations in Membrane Science for Sustainable Systems

S. Oyama, *Organizer*
S. M. Stagg-Williams, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 74. Correlation between pyrolysis atmosphere and carbon molecular sieve membrane performance properties. M. Kiyono, **W. J. Koros**, P. J. Williams

2:20 75. Gas transport properties of poly acrylate/clay nanocomposites prepared via emulsion polymerization. **J. Herrera**, E. Marand, Z. Sedlakova

2:45 76. On a membrane-based process for CO_2 capture from internal combustion vehicles. C.-H. Nicolas, A. Alshebani, **M. Pera-Titus**, J.-P. Roumégoux, T. Schiestel, S. Miachon, J.-A. Dalmon

3:10 Intermission.

3:20 77. Correlations between pore structure, functional layer chemistry and architecture, and separation performance of advanced membrane adsorbers. **M. Ulbricht**, C. Kaul, C. Kuhn, S. Schwark, F. Tomicki, J. Wang, Q. Yang

4:05 78. Increase of the product recovery of Clostridium acetobutylicum fermentation product by pervaporation. **P. Izák**, V. Jarmarová, K. Schwarz, W. Ruth, H. Bahl, U. Kragl

4:30 79. High temperature gas separations using high performance polymers. **J. R. Klaehn**, C. J. Orme, T. A. Luther, **E. S. Peterson**, J. M. Urban-Klaehn

4:55 80. High throughput combinatorial method for choosing membrane polymer chemistry: Solvents and binary systems. S. H. Yun, M. Gu, C. Kilduff, **G. Belfort**

5:20 81. Pervaporation performance of PEG/PVDF composite membrane for separating cyclohexanol/cyclohexane mixtures. M. Huang, **C. Zeng**, J. Chen, J. Li

Section E

InterContinental San Francisco
Grand Ballroom B

CO_2 Capture, Conversion and Utilization

Catalytic and Electrochemical Conversion of CO_2

V. S.-Y. Lin, and B.-L. Su, *Organizers*
G. Centi, *Presiding*

1:30 82. Electrochemical conversion of carbon dioxide into useful products: Approaches and challenges. **N. Sridhar**, Y. Zhai, A. Agarwal, E. Hektor, T. Myhrvold, L. Chiacchiarelli, G. S. Frankel

2:05 83. Carbon dioxide as a building block for organic urea compounds, carbamates, and carbonates. A. Ion, C. Van Doorslaer, P. A. Jacobs, V. Parvulescu, **D. E. De Vos**

2:30 84. Recent progress in CO_2 conversion to oxygen-rich compounds. **T. Sakakura**, J.-C. Choi, H. Yasuda, T. Takahashi, K. Kohno, S. Kitazume, L.-N. He

2:55 85. Catalytic production of methane from CO_2 and H_2 at low temperature and low pressure: A new breakthrough in the knowledge to recycle the CO_2 . **M. Jacquemin**, A. Beuls, P. Ruiz

3:15 Intermission.

3:25 86. Hydrogenation of carbon dioxide to methanol over multicomponent copper-based catalysts. **S. Natesakhawat**, B. Morreale

3:45 87. Theoretical modeling of carbonate formation in dehydrated alkaline earth zeolites. A. Larin, A. Rybakov, G. M. Zhidomirov, A. Mace, A. Laaksonen, **D. P. Vercauteren**

4:05 88. New catalysts for the photochemical reduction of CO_2 in supercritical CO_2. **D. C. Grills**, M. D. Doherty, E. Fujita

4:25 89. Promotional effect of alkaline earth over Ni/La_2O_3 catalysts for hydrogen production via CO_2 reforming of methane. K. Sutthiumporn, **S. Kawi**

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Peter C. Stair

From Surface Science to Heterogeneous Catalysis: Understanding Practical Catalysts

Sponsored by CATL (probationary), Cosponsored by FUEL and PETR

Catalysis for Sustainability

CO2 Conversion and Utilization

Sponsored by CATL (probationary), Cosponsored by FUEL and PETR

Catalysis for Sustainability

Photocatalysis for Fuel Synthesis: Molecular and Hybrid Systems

Sponsored by CATL (probationary), Cosponsored by FUEL

MONDAY MORNING

Section A

InterContinental San Francisco
Grand Ballroom A

Green Chemistry on Fuels of the Future

Catalysts and Nanomaterials

M. Dong, R. Glaeser, and C. Liu, *Organizers*
S.-E. Park, *Presiding*
W.-L. Jang, *Organizer, Presiding*

8:30 90. Development of metal decorated carbon nanotubes-supported catalysts for microchannel methanation reactor. **R. L. Vander Wal**, J. Novak, C.-H. Hunag

8:50 91. Fischer-Tropsch products from compact reactor and high-temperature Iron catalyst. **A. Czernichowski**, M. Czernichowski

9:10 92. Inducing metal-support interaction via non-thermal plasma technology for catalyst design and fuel synthesis. Y. Li, **B. W.-L. Jang**

9:30 93. Synthesis of solar fuels by novel photoelectrocatalytic approach. **G. Centi**, **S. Perathoner**, R. Passalacqua, C. Ampelli

9:50 94. Role of catalysis in green chemistry for fuel processing and CO_2 control. **C. Song**

10:35 Intermission.

10:45 95. Insights into structure-sensitive reactions using model supported nanoparticles: Reaction kinetics and PM-IRAS studies at near atmospheric pressures. S. M. McClure, M. Lundwall, **D. W. Goodman**

11:30 96. Mesoporous carbon nitride materials as metal-free oxidation catalyst. **S.-E. Park**, B.-H. Min, E. A. Prasetyanto, H.-U. Seo

11:50 97. TiO_2-TiC composite with porous shell-core structure for the support of anode electrocatalyst in proton exchange membrane water electrolyzer (PEMWE). **S. Sui**, W. Yan, S. Li

12:10 98. Preferential oxidation of CO in H2-rich feed over unsupported nanocomposite and structured carbon nanofiber supported Cu-CeO_2 catalysts. **T. Zhao**, Y. Yu, D. Chen, M. Ronning

Section B

InterContinental San Francisco
Union Square

Solar Cells and Solar Fuels

Organic Photovotaics

H. Jai, Y. Lu, L. Sun and D. Wang, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 99. Multi-source/component spray coating for polymer solar cells. **Y. Yang**, L.-M. Chen, Z. Hong, W. L. Kwan, B. Lei

9:00 100. Using nanoscale self-organization and interfacial control to improve performance in semiconducting polymer-based photovoltaics. A. L. Ayzner, C. Tassone, R. Kennedy, A. P.-Z. Clark, C. Shi, B. de Villers, Y. Rubin, B. J. Schwartz, **S. H. Tolbert**

9:30 101. Redox-tunable perfluoroalkylfullerene-based polymers with highly variable donor/acceptor domain morphologies for opv active layers. N. C. Escudé, B. W. Larson, W. L. Rance, M. J. Wells, J. B. Whitaker, T. S. Bailey, O. V. Boltalina, E. Y. Chen, N. Kopidakis, **S. H. Strauss**

10:00 102. Facile synthesis of asymmetric perylene tetra-carboxylic diimide with functional nanoparticle side chain potentially useful in photovoltaic and study on their self-assembly behavior. **B. Sun**, W.-B. Zhang, K. Li, C.-L. Wang, X. Ren, S. Yang, Y. Tu, M. Guo, **M. Zhu**, S. Z. D. Cheng

10:20 Intermission.

10:30 103. Highly conductive transparent electrode materials using partially aligned carbon nanotube networks. **M. C. LeMieux**, A. Virkar, Z. Bao

10:50 104. Future challenges for the industry of organic photovoltaics. **G. Dennler**, R. Gaudiana

11:20 105. Plastic solar cells: The vision of Sukant Tripathy has become reality. **A. J. Heeger**

Section C

InterContinental San Francisco
Grand Ballroom C

Theory and Simulation in Energy Production and Utilization

Cosponsored by PHYS
Q. Ge, and J.-G. Wang, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 106. Stability of hydrogen clathrates of ammonia borane. **M. Gutowski**, A. V. Abramov

9:20 107. Electric field enhanced hydrogen storage on polarizable materials substrates. **Q. Sun**, J. Zhou, Q. Wang, P. Jena

10:05 Intermission.

10:15 108. Ab initio modeling of microscopic structures and processes in hydrogen storage and electrochemical energy conversion. **A. Gross**

11:00 109. Design and development of novel materials for hydrogen storage. **H. Cheng**

11:45 110. Computational screening and design of complex materials for hydrogen storage and solid electrolytes. **T. Vegge**, J. S. Hummelshøj, J. B. Maronsson, J. S. G. Myrdal, S. Lysgaard

Section D

InterContinental San Francisco
Grand Ballroom B

Correlations in Membrane Science for Sustainable Systems

S. M. Stagg-Williams, *Organizer*
S. Oyama, *Organizer, Presiding*

8:30 111. High performance ultrafiltration membranes: Pore geometry and charge effects. **A. L. Zydney**

9:15 112. Highly porous uniform pore size membranes for ultrafiltration. X. Wang, S. M. Husson, X. Qian, **S. R. Wickramasinghe**

9:40 113. Theory of hydrogen permeance in a hydrothermally stable silica-alumina membrane . **P. Hacarlioglu**, D. Lee, Y. Gu, T. S. Oyama

10:05 114. Preparation of silica membranes by sol-gel processing and permeation characteristics of gaseous molecules through microporous silica membranes with controlled pore sizes and surface chemistry . T. Tsuru, **M. Kanezashi**, R. Igi, A. Yamamoto, T. Yoshioka

10:30 Break.

10:40 115. Prospects for energy saving of distillation process with microporous membrane. **M. Matsukata**, K.-I. Sawamura, Y. Sekine, E. Kikuchi

11:25 116. CO_2 permeability and mixed gas CO_2/H_2 selectivity of membranes composed of CO_2-philic oligomers. **M. K. Barillas**, **R. M. Enick**, D. Luebke, B. Morreale

11:50 117. Concentrating protein solution by a new crossflow electro-ultrafiltration process. W. Song, Y. Su, X. Chen, **Y. Wan**

Sustainability of the Sugar and Sugar-Ethanol Industries

Sponsored by CARB, Cosponsored by AGFD, CELL and FUEL

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Robert J. Madix

From Surface Science to Heterogeneous Catalysis: Catalytic Reactions on Well-Defined Surfaces

Sponsored by CATL (probationary), Cosponsored by COLL, FUEL and PETR

Ipatieff Prize: Symposium in Honor of Christopher W. Jones

Sponsored by CATL (probationary), Cosponsored by FUEL and PETR

Supported Molecular Catalysts

Sponsored by CATL (probationary), Cosponsored by COLL, FUEL and PETR

MONDAY AFTERNOON

Section A

InterContinental San Francisco
Grand Ballroom A

Green Chemistry on Fuels of the Future

Catalysts and Nanomaterials

M. Dong, W.-L. Jang, and C. Liu, *Organizers*
S. Moon, *Presiding*
R. Glaeser, *Organizer, Presiding*

1:30 118. Researches for the effective removal of sulfur from refractory compounds. S. I. Lee, A. Cho, **S. H. Moon**

2:15 119. Active sites on supported Pt and PtPd catalysts for deep hydrotreating. **J. Lercher**

2:35 120. Preparation of nickel-loaded zirconias. A. Peters, M. Lutecki, **R. Glaeser**

2:55 121. Nature of the aluminum phases in aluminum oxide-coated titanium oxide particles. **E. W. Hagaman**, J. Jiao, Z. Ma, H. Yin, S. Dai

3:15 122. Hydrogenolysis of glycerol by Cu supported on γ-Al_2O_3 catalysts. S. Hao, W. Peng, N. Zhao, F. Xiao, **W. Wei**, **Y. Sun**

3:35 Intermission.

3:45 123. Diesel-length aldehydes from supercritical Fischer Tropsch Synthesis on an iron catalyst. **E. Durham**, C. B. Roberts

4:05 124. Fe doped La_2O_3 catalyst for oxidative coupling of methane. **K. Tanaka**, Y. Sekine, M. Matsukata, E. Kikuchi

4:25 125. Chiral oxidation reaction over single-site heterogenized biomimetic amino acid complexes catalyst. **E. A. Prasetyanto**, M. B. Ansari, S.-E. Park

4:45 126. Hydrodenitrogenation performance of TiO_2- and CeO_2-promoted Ni_2P catalysts. **X. Li**, Z. Sun, A. Wang, Y. Wang

Section B

InterContinental San Francisco
Grand Ballroom C

Solar Cells and Solar Fuels

DSSC

H. Jai, Y. Lu, L. Sun and D. Wang, *Organizers, Presiding*

1:30 127. Efficient energy harvesting using hybrid structures and hybrid cells. **Z. Z. L. Wang**

2:00 128. First-row transition metal-based chromophores for dye-sensitized solar cells: Fundamental issues and application in solar energy conversion. **J. K. McCusker**

2:30 129. Titanium dioxide aggregates used in dye-sensitized solar cells for conversion efficiency enhancement. Q. Zhang, **G. Cao**

3:00 130. Optimization of dye-sensitized solar cells based on organic dyes. **M. Gorlov**, A. Lindborg, M. Karlsson, H. Tian, **L. Sun**

3:20 Intermission.

3:30 131. Photoelectrodes of dye-sensitized solar cells based on 1D TiO_2 nanomaterial assembly. **H. Fu**

4:00 132. Photoelectrochemistry of oxide semiconductors for dye-sensitized solar cells. G. Natu, **Y. Wu**

4:30 133. Donor-acceptor nanostructures for solar energy conversion. **H. Imahori**

4:50 134. Strategy toward two bands tandem organic dye sensitized solar cell. **X. Yang**, Y. Hao, C. Teng, L. Sun

Section C

InterContinental San Francisco
Union Square

Theory and Simulation in Energy Production and Utilization

Cosponsored by PHYS
Q. Ge and J.-G. Wang, *Organizers, Presiding*

1:30 135. Bioinspired catalyst/electrode system for hydrogen production. F. Zipoli, M. H. Cohen, R. Car, **A. Selloni**

2:15 136. Electrocatalysis from first principles. **M. Neurock**

3:00 137. Mechanism and life-cycle emissions from synthetic fuels. **O. Inderwildi**

3:45 138. Generalized Monte-Carlo based framework for simulating catalytic and electrocatalytic systems for energy applications. V. Viswanathan, **F. Y.-F. Wang**, H. Pitsch

InterContinental San Francisco
Grand Ballroom B

Correlations in Membrane Science for Sustainable Systems

Cosponsored by PETR
S. Oyama and S. Stagg-Williams, *Organizers, Presiding*
S. Oyama, *Presiding*

1:30 139. Using first principles modeling to accelerate development of dense metal membranes for high temperature hydrogen separation. **D. S. Sholl**, S. Hao, L. Semidey-Flecha, C. Ling, S. G. Kang

2:15 140. Effect of mass transfer on Cu plating rate and deposition morphology for Pd/Cu alloy membranes for hydrogen separation. N. Pomerantz, **Y. H. Ma**

2:40 141. Role of the surface nanostructure on the performances and stability of H_2 separation thin-film membrane. **G. Centi**, S. Perathoner, S. Abate

3:05 142. Hydrogen production via composite palladium membranes with long-term selectivity stability. **M. E. Ayturk**, Y. H. Ma

3:30 Break.

3:40 143. Investigation of H_2 and H_2S interactions on Pd-Nb and Pd-Cu alloy surfaces for hydrogen separation. **E. Ozdogan**, J. Wilcox

4:05 144. Effect of H_2S concentration on hydrogen permeation of a composite Pd/Au hydrogen separation membrane prepared by galvanic displacement. **C.-H. Chen**, Y.-H. Ma

4:30 145. Surface alloys for control of sulfur corrosion in Pd-based H_2 separation membranes. **C. O'Brien**, B. Howard, J. Miller, B. Morreale, A. Gellman

4:55 146. Membrane separation of ethanol from gasoline mixed with bio-ethanol. **A. Yamasaki**, T. Tanaka, Y. Ueda, T. Kojima, S. Satokawa

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Peter C. Stair

From Surface Science to Heterogeneous Catalysis: Catalytic Reactions on Well-Defined Surfaces

Sponsored by CATL (probationary), Cosponsored by FUEL and PETR

Ipatieff Prize: Symposium in Honor of Christopher W. Jones

Sponsored by CATL (probationary), Cosponsored by FUEL and PETR

Supported Molecular Catalysts

Sponsored by CATL (probationary), Cosponsored by COLL, FUEL and PETR

MONDAY EVENING

Section A

The Moscone Center
Hall D

Sci-Mix

V. Subramani, *Organizer*
C. Liu, *Organizer, Presiding*

8:00 - 10:00
14, 19, 36, 39, 43, 47, 49, 51, 55, 61, 63, 70, 76, 90, 92, 112, 127, 143. See previous listings.

203, 209, 213, 220, 221, 238, 246, 255, 258, 263, 264, 272, 273, 276, 280, 296, 327, 330, 331, 338, 347, 370. See subsequent listings.

Section A

The Moscone Center
Hall D

Advances in Fuel Science and Technology

C. Liu, *Organizer*
H. Hu, and S. Kado, *Presiding*
S.-E. Park, *Organizer, Presiding*

8:00 - 10:00
147. RICH®-II technology for improving cetane number of FCC-LCO. **J. Xin**, H. Nie, M. Li, S. Dong, Y. Zhang, Z. Hu, D. Li

148. Reformate impurity effects on high temperature PBI based fuel cell membranes. **G. Qian**, S. Yu, B. Benicewicz

149. Anhydrous proton conducting organic–inorganic hybrid membranes prepared from tetraethoxysilane/methyltriethoxysilane/trimethylphosphate and 1-butyl-3 methylimidazolium tetrafluoroborate for H_2/O_2 fuel cells. **G. Lakshminarayana**, M. Nogami

150. Investigation of back electron transfer control in Aminoborane derivatives using dynamic NMR. **D. Hornyak**, A. Nguyen, I. Parchamazad

151. Analytic study of petroleum marker using HPLC. **Y.-K. Lim**, J.-R. Kim, E. S. Yim, D.-K. Kim, S.-C.

Shin, C.-S. Jung

152. Determination of monosaccharides in acid-hydrolyzed corn stover using HPAE-PAD. **R. A. Kornfeld**, V. P. Hanko, L. L. Lopez, J. S. Rohrer

153. Improved method to predict the flash points of hydrocarbons. **F. A. Carroll**, C.-Y. Lin, F. H. Quina

154. Determination of cations in biodiesel fuels by cation exchange ion chromatography with suppressed conductivity detection. **D. C. Hurum**, B. M. De Borba, L. L. Lopez, J. S. Rohrer

155. Synergetic study on co-pyrolysis of biomass and coal in wire mesh reactor. **X. Guo**, H. Zhu, C. Zeng, B. Eiteneer, S. D. Sanborn

156. Properties of metal-water interfaces studied from first principles. **S. Schnur**, A. Gross

157. Comparison of growth and lipid production by use of fluorimetric assays in non-triggered and lipid-triggered Neochloris oleoabundans algal cultures. **J. V. Volponi**, H. Wu, S. Singh

158. Selective removal of acetylenes from olefin mixtures through specific physicochemical interactions of ionic liquids with acetylenes. **H. S. Kim**, J. M. Lee, J. Palgunadi, M. Cheong

159. Analog between zeolite and gas discharge plasma. Y. Zhang, **C.-J. Liu**

160. Potential photochromic proton exchange membrane as an alternative for PEMFCs. **F. P. Rodríguez-Rivera**, M. Pagán-Ortiz, J. J. Chambers

161. Toward the development of a laccase airbreathing bioelectrode with anthracene modified chitosan. **Z. Caban**, S. Minteer, A. Demchemko, A. Ramakrishnan

162. Desulfurization of high sulfur coal by mild pyrolysis combination with magnetic separation. **L. Quanrun**, X. Hao, W. Can

163. Effect of dispersants on lignite char water slurry. P. Zhang, **H. Hu**, L. Jin, Y. Fan

164. Catalytic oxidation behavior over ti containing mesoporous tud-1. **S.-M. Jeong**, N. Jiang, S.-E. Park

165. Role of mesoporosity of hierarchical mesoporous ZSM-5 in aid catalysis. **H. Jin**, N. Jiang, E. A. Prasetyanto, J. Cejka, S.-E. Park

166. High surface area mesoporous TiO_2-ZrO_2: Amorphisation of TiO_2-ZrO_2 by alkali metal doping. **A. Burri**, N. Jiang, S.-E. Park

167. Oxidation of elemental mercury by using NaClOx (x=1,2,3) injection. **D. N. Shin**, J. Kim, Y. Byun, D. J. Koh

168. *Clostridium Acetobutylicum* NADH-dependent butanol dehydrogenase for use in butanol bioproduction. **S. Besic**, S. D. Minteer

169. Preparation of carbon catalysts for PEFC from polyimides as precursors. **M. Taniguchi**, M. Chokai, S. Moriya, K. Matsubayashi, T. Shinoda, Y. Nabae, S. Kuroki, T. Hayakawa, M.-A. Kakimoto, J. Ozaki, S. Miyata

170. Investigations into CO_2 selectivity and storage capacity of metal organic frameworks: A molecular

simulation study. **P. G. Boyd**, S. Alavi, T. K. Woo, D. van Rijswijk

171. Synthesis and characterization of a novel Zn-based MOF. **J. Kolev**, C. G. Collison

172. Design and optimization of sugar powered biofuel cells based on PQQ dependent enzymes. **S. Xu**, S. D. Minteer

173. Kinetic properties of larger hydrocarbon fuel molecules and radicals under pyrolysis. **W. Tsang**

174. Quantitative determination of oxygenate additives in gasoline and diesel fuels by infrared spectroscopy. **J. A. Boachie**, B. G. Ooi, L. Bolin, N. S. Chong

175. Development of metal (Ta,Nb)/ceramic and cellulose acetate membranes for Cu-Ni-Ce/alumina WGS catalytic reactor. **N. V. Seetala**, U. Siriwardane, T. V. Kudale, R. Forester, A. Pokharel

176. Long-term air stability of organically-capped aluminum nanoparticles. **M. A. Burgers**, **C. D. Oberle**, S. W. Buckner, C. E. Bunker, P. A. Jelliss, E. A. Guliants, D. W. Hammerstroem, V. Kalugotla, S. W. Chung

177. Rapid control of hydrogen permeability through palladium membrane by microwave heating. **M. Nishioka**, K. Sato, M. Kasai, H. Higashi, T. Inoue, Y. Hasegawa, Y. Wakui, T. M. Suzuki, F. Mizukami, S. Hamakawa

178. Small Angle X-ray scattering (SAXS) measurements of nanomaterials. **A. Tripathi**, T. F. McNulty

179. Catalytic cracking of sulfone compounds in ODS diesel over Cs-mesoporous catalysts. **H. Kim**, Y. J. Lee, S.-Y. Jeong, K.-E. Jeong, Y.-K. Park, Y. S. Ko, J.-K. Jeon

180. Effects of oxygenate additives in reducing air toxics from the exhaust emissions of generators fueled by diesel and gasoline. **L. Bolin**, N.-S. Chong, F. Ahmed, P. Schine, B. G. Ooi

181. Advanced gas sorption techniques in energy storage applications. **A. A. Levchenko**, P. Le Parlouer, E. Wirth, K. Gross

182. Study in biodiesel's oxadative stability: A long term pilot scale study. **M. J. Fischer**, I. Abou-Nemeh

183. Hydrogen fuel gas production using high pressure water. **W. Eltringham**

184. Thermodynamic driving forces for post-gasification carbon deposition. **C. J. Pope**, P. A. Marrone, B. V. Yeh

185. Analysis of aromatic carbon in ZrCl4 using UV spectroscopy. **S. Barrett**, R. Maass, C. Jones, E. Walker

186. Polymer brush induced reconstructed morphology of ABC triblock copolymer thin film. **R. Wang**, C. Xu

187. Relation between double layer capacitance and porosity structure of carbon aerogels based on ionic liquid electrolyte. Q. Wang, L. Jin, **H. Hu**, Y. He

188. Study on coliquefying reactivity of coals with cornstalk. **X. Guo**, F. Zhang, S. Zhong, S. Mao, Y. Wang, D. Xu

189. Characterization of iron containing AlPO-5 zeolites for selective catalytic reduction of N_2O with CH_4 in the presence of steam. **D.-G. Cheng**

190. Comparative study of Fe-Mo bimetallic carbide catalysts with different preparation methods for higher alcohols synthesis. N. Wang, K. Fang, D. Jiang, M. Lin, D. Li, **Y. Sun**

191. Application of SHELL's all hydrogen catalysts on the manufacturing of 8# paraffinic base HVIP lube base oil. **X. Liu**, J. Sun

192. Reduction-oxidation-reduction(ROR) activated method for Co-based FT catalysts. S. Mu, D. Li, B. Hou, L. Jia, J. Chen, **Y. Sun**

193. Relationship of the molecular structure and biological activity of humic acid. **C. Zhang**

194. Plasma-assisted selective partial oxidation of tars and other pollutants in producer gases. **A. Czernichowski**, P. Czernichowski

195. Oxy-CO_2 reforming of methane using Al-La based Ni catalysts with formation of stable $LaAlO_3$ s structural support. **Y. Kathiraser**, K. Sutthiumporn, K. Sibudjing

196. Tunable preparation and CO_2 capture of colloidal layered double hydroxides spheres. K. Ye, **S. Xu**

197. Solubility of sulfur dioxide in concentrated brine. P. Zhu, H. Wang, **X. Li**

198. Catalytic trimerization of n-butene over Ni-containing HZSM-5 with high Si/Al ratio. **X. Zhang**

TUESDAY MORNING

Section A

InterContinental San Francisco
InterContinental Ballroom B

Green Chemistry on Fuels of the Future

Alternative Feedstocks

D. Chen, *Presiding*
W.-L. Jang, *Organizer, Presiding*

8:30 199. Enzymatic Transesterification of Oil and Methanol: Activity and Stability Study of Enzyme Immobilized Passivated SBA-15. W. Thitsartarn, **S. Kawi**

8:50 200. Furanics: Promising results from ESC tests with a DAF Truck diesel engine. **E. DeJong**, D. DenOuden, G.-J. Gruter

9:10 201. Highly efficient hydrogen production from biomass. L. He, **D. Chen**

9:30 202. All about biorefining. **A. J. Ragauskas**

9:50 203. Transesterification of oil to biodiesel by using calcium diglyceroxide as solid base catalysts. Z. Huang, Y. He, D. Zhou, **S. Zhang**, **J. Chen**

10:10 Intermission.

10:20 204. Catalytic conversion of biomass: Options and challenges. **W. Leitner**

11:05 205. Physical and chemical characteristics of as produced and aged pyrolysis oils produced from woody biomass feedstocks and their optimization towards the production of a truly green syn gas. **A. M. Herring**, J. V. Ortega, A. Renehan

11:25 206. Evaluation of pretreatment methods in the production of ethanol from cattail leaves: Application in biochemistry. **E. N. Wreh**

11:45 207. Bifunction of Ti^{3+} in TiO_2/Cu_2O composite: Degradation of organic pollutant and production of H_2 from water splitting under visible light. L. Xiong, L. Ren, Y. Deng, F. Yang, **Y. Yu**

Section C

InterContinental San Francisco
InterContinental Ballroom C

Theory and Simulation in Energy Production and Utilization

Cosponsored by PHYS
Q. Ge and J.-G. Wang, *Organizers, Presiding*

8:30 208. Selective hydrogenolysis of small oxygenates on transition metal surfaces. **Y. Xu**

9:15 209. Fischer-Tropsch synthesis on iron and cobalt carbides: A density functional theory study. **P. Hu**

10:00 210. DFT modeling of rare earth metal oxide for catalysis and energy production. **X. Gong**, H. Wang, H. Li, P. Hu, G. Lu

10:30 Intermission.

10:40 211. Theoretical investigation of NO_x storage on γ-Al_2O_3-supported barium oxide materials. **D. Mei**, Q. Ge, J. H. Kwak, J. Szanyi, C. H. F. Peden

11:25 212. Multi-scaling study of adsorption and desorption of methanol on TiO2(110) surface. K. Sun, **W.-X. Li**

Section D

InterContinental San Francisco
Grand Ballroom A

Correlations in Membrane Science for Sustainable Systems

S. Stagg-Williams, *Organizer*
S. Oyama, *Organizer, Presiding*

8:30 213. Critical factors affecting oxygen permeation through dual-phase membranes. X. Zhu, **W. Yang**

9:15 214. $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_x$ asymmetric oxygen-permeable ceramic membrane for CO_2 reforming and

partial oxidation of methane. **Q. Jiang**, K. J. Nordheden, **S. M. Stagg-Williams**

9:40 215. Fabrication of oxide ceramic multilayer membranes. **V. V. Zyryanov**

10:05 Break.

10:15 216. Zeolite membranes for gas separation: Relationship between structure and gas permeation properties. **J. Y. S. Lin**

11:00 217. Thermotropic liquid-crystal polymer membranes for vapor-phase separations. **F. H. Rabie**, S. Martin, E. Marand

11:25 218. Mesoscale simulation of nanosegregation in permselective polyelectrolyte membranes. **A. Vishnyakov**, S. Yang, A. V. Neimark

Section E

InterContinental San Francisco
Grand Ballroom E

Hydrogen Storage

Boron Containing Materials: Borohydrides

Y. Hu, *Organizer*
T. Gennett, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 219. Achievements and perspectives of the US National Program on Hydrogen Storage R. **C. Read**, B. Bowman, M. Gardiner, G. Ordaz, N. Stetson, S. Dillich

8:55 220. Hydrogen storage in alkali and alkaline earth borohydrides: Probing the role of intermediate species. **V. Stavila**, R. J. Newhouse, S.-J. Hwang, M. Ulutagay-Kartin, J.-H. Her, T. J. Udovic

9:25 221. Ammonia borane and a new ammonia borane-hydrogen compound at high pressure. **Y. Lin**, V. Drozd, J. Chen, L. L. Daemen, H.-K. Mao, W. L. Mao

9:45 222. Bisboranohypophosphite salts as reversible hydrogen storage media. **M. R. Anstey**, J. G. Cordaro

10:05 223. Hydrogen generation from small molecules using bifunctional Ruthenium complexes. **A. Friedrich**, M. Drees, J. Schmedt auf der Günne, S. Schneider

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Robert J. Madix

From Surface Science to Heterogeneous Catalysis: Oxygen-Assisted Reactions on Metallic Gold and Other Nobel Metals

Sponsored by CATL (probationary), Cosponsored by COLL, FUEL and PETR

Supported Molecular Catalysts

Sponsored by CATL (probationary), Cosponsored by COLL, FUEL and PETR

TUESDAY AFTERNOON

Section A

InterContinental San Francisco
Telegraph Hill

Green Chemistry on Fuels of the Future

Alternative Feedstocks

W.-L. Jang, *Organizer*
R. Glaeser, and G. Huber, *Presiding*

1:30 224. Low temperature hydrothermal conversion of macroalgae *Enteromorpha prolifera* to bio-oil. D. Zhou, L. Zhang, **S. Zhang**, H. Fu, **J. Chen**

1:50 225. Development of CPOX monolith catalyst for efficient GTL process. **S. Kado**, K.-I. Imagawa, A. Kiryu, F. Yagi, T. Minami, K.-I. Kawazuishi, H. Kawai, K. Tomishige, A. Nakamura, Y. Suehiro

2:10 226. Integrated process for depolymerization of lignocellulosic materials: Maximizing carbon efficiency by combining hydrolysis with pyrolysis. **J. Jae**, G. A. Tompsett, Y.-C. Lin, T. R. Carlson, J. Shen, T. Zhang, B. Yang, C. E. Wyman, W. C. Conner, G. W. Huber

2:30 227. One-pot synthesis of alcohols from olefins catalyzed by rhodium and ruthenium complexes. **J. Zakzeski**, H. R. Lee, Y. L. Leung, A. T. Bell

2:50 228. New navy fuels from 2-ethyl-1-hexene. **B. G. Harvey**, R. L. Quintana

3:10 Intermission.

3:20 229. Green gasoline and petrochemicals from lignocellulosic biomass by pyrolysis based technologies. **G. W. Huber**

4:05 230. Glycerol derivatives as fuel additives for gasoline and biodiesel. **C. J. A. Mota**, C. X. da Silva, B. P. Pinto, R. Lorençatto, V. L. C. Gonçalves

4:25 231. Biodiesel catalyst made from fish scale. **X. Zheng**, D. Huang, Y. Xue, L. Fu

4:45 232. Photoreduction of carbon dioxide to acetaldehyde under a series of temperatures and pressures. **T. Xulong**, C. Guangjin, F. Jing, L. Haili

Section C

InterContinental San Francisco
InterContinental Ballroom A

Theory and Simulation in Energy Production and Utilization

Q. Ge and J.-G. Wang, *Organizers, Presiding*

1:30 233. Mechanistic study of ethylene conversion to ethylidyne on M(111) (M = Pd, Pt) with DFT and kinetic Monte Carlo simulations. H. A. Aleksandrov, Z.-J. Zhao, D. Basaran, L. V. Moskaleva, Z.-X. Chen, D. Mei, **N. Roesch**

2:15 234. First principles description of dark multi-exciton states involved in MEG of carbon nanotubes. P. M. Zimmerman, Z. Zhang, **C. B. Musgrave**

2:35 235. Energy and nanomaterials: Interfacial synergy. **R. L. Vander Wal**

2:55 236. Photo-electrochemical water splitting by GaN, InGaN, and ZnO: A density functional theory study. **P. G. Moses**, C. G. Van de Walle

3:15 Intermission.

3:25 237. Photon induced electron excitation and transfer in MK and modified MK dyes for dye-sensitized solar cells (DSSCs). **L. Wang**, G. A. Hudson

4:10 238. Mesoporous titania with TiO_2(B): Synthesis, features, and applications. **X. Lu**, W. Li, W. Liu, Y. Bai, C. Liu, Z. Yang, X. Feng, K.-Y. Chan, J. Wang

4:55 239. First principles description of two hydrogen transfer for CO_2 reduction. **P. M. Zimmerman**, Z. Zhang, C. B. Musgrave

Section D

InterContinental San Francisco
Twin Peaks

Correlations in Membrane Science for Sustainable Systems

S. Oyama, *Presiding*
S. Stagg-Wiliams, *Organizer, Presiding*

1:30 240. Correlations in zeolite and ionic liquid membrane performance. **R. D. Noble**, D. L. Gin, J. L. Falconer, S. G. Sorenson, J. R. Smyth, Y. C. Hudiono

2:15 241. Proton-conducting organic molecules as separator materials for fuel cell applications. **L. Jiménez-García**, A. Kaltbeitzel, V. Enkelmann, J. S. Gutmann, M. Klapper, K. Müllen

2:40 242. Metal ion exchange method for assignment of IR peaks in ion exchange membranes. **D. Kumari**, A. Rivera, E. Smotkin

3:05 243. Sol-gel polymerization of bridged polysilsesquioxanes to afford membranes for gas separations. **Z.**

Li, D. A. Loy

3:30 244. 1D and 2D modeling studies of methane steam reforming in a membrane reactor. **P. Hacarlioglu**, T. S. Oyama

3:55 Concluding Remarks.

Section E

InterContinental San Francisco
Grand Ballroom B

Hydrogen Storage

Boron Containing Materials: B-doped Carbon Materials

T. Gennett, and Y. Hu, *Organizers*
P. Parilla, *Presiding*

1:00 245. Super-activated carbon containing substitutional boron for hydrogen storage. Y. Jeong, **T. C. M. Chung**

1:30 246. Boron doped high surface area carbon for hydrogen storage. **J. Bult**, J. Blackburn, C. Engtrakul, L. Simpson, T. Gennett

1:50 247. High-throughput detection of hydrogen sorption on carbon-based materials using Raman and infrared spectroscopies. **J.-D. R. Rocha**, D. Zhao, J. B. Bult, C. Engtrakul, K. J. O'Neill, J. G. Barker, L. J. Simpson, H.-C. Zhou, M. J. Heben, J. L. Blackburn

2:10 248. Stabilization of lithium atoms on supported BC_x materials for novel hydrogen sorption materials. **C. Engtrakul**, J. L. Blackburn, J. B. Bult, K. J. O'Neill, J. G. Barker, J.-D. R. Rocha, T. Gennett, L. J. Simpson

2:30 Intermission.

Section E

InterContinental San Francisco
Grand Ballroom B

Hydrogen Storage

Structured Organic and Inorganic Materials

T. Gennett, *Organizer*
Y. Hu, *Organizer, Presiding*

2:40 249. Renewable carbohydrate is a high-energy density hydrogen carrier, better than methanol. **Y.-H. P. Zhang**

3:10 250. Porous organic networks and their hydrogen uptake properties. **S. Yuan**, S. Kirklin, B. Dorney, D.-

J. Liu, L. Yu

3:30 251. Theory and simulation on hydrogen adsorption in MOFs, COFs, and ZIFs. **S. S. Han**, W. A. Goddard

3:50 252. Effect of atomic hydrogen adsorption on structure of metal organic frameworks. **Y. H. Hu**

4:10 253. Investigation of metal hydride nanoparticles templated in porous frameworks. **R. K. Bhakta**, J. L. Herberg, A. M. Highley, R. Behrens, **M. D. Allendorf**

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Peter C. Stair

From Surface Science to Heterogeneous Catalysis: From Metals to Oxides and Back

Sponsored by CATL (probationary), Cosponsored by FUEL and PETR

Ipatieff Prize: Symposium in Honor of Christopher W. Jones

Sponsored by CATL (probationary), Cosponsored by FUEL and PETR

WEDNESDAY MORNING

Section A

InterContinental San Francisco
Grand Ballroom A

Green Chemistry on Fuels of the Future

Alternative Processes

M.B. Chang, and A. Stark, *Presiding*
W.-L. Jang, *Organizer, Presiding*

8:30 254. Direct dissolution and NMR analysis of the plant cell walls via perdeuterated pyridinium-based ionic liquid. **N. Jiang**, Y. Pu, R. Samuel, A. J. Ragauskas

8:50 255. Overview of effective H_2 production via plasma catalysis. **M. B. Chang**, H. L. Chen, Y. Chao, H. M. Lee

9:10 256. Biogas valorization by non-thermal plasma process.. V. Goujard, **C. Batiot-Dupeyrat**, J.-M. Tatibouet

9:30 257. Production of zero-oxygen hydrocarbons from biomass-based bio-oil. **P. H. Steele**, S. K. Gajjela

9:50 258. Conversion of lignocellulosic biomass by a sequential combination of organic acid and base treatments. **U. Wongsiriwan**, Y. Noda, P. Prasassarakich, Y. Yeboah, C. Song

10:10 259. Hydrothermal and solvothermal processes for renewable fuels. **P. E. Savage**

10:30 Intermission.

10:40 260. Ionic liquids in the biorefinery: A critical assessment of their potential. **A. Stark**

11:25 261. Improved enzymatic bioprocessing of cotton waste using a low level, uniform ultrasound field. **M. W. Easson**, B. Condon, V. Yachmenev, A. Lambert, C. Delhom, J. Smith

11:45 262. Two-step catalytic conversion of glucose to 2,5-dimethylfuran in ionic liquids. **M. Chidambaram**, A. T. Bell

12:05 263. Advanced material sytems/processes for green chemistry: Microfluidic synthesis. **K. Choi**

Section B

InterContinental San Francisco
InterContinental Ballroom A

Solar Cells and Solar Fuels

Water Oxidation

H. Jia, Y. Lu, L. Sun, and D. Wang, *Organizers, Presiding*

8:15 264. Visible light driven water oxidation catalyzed by molecular Ru complexes bearing carboxylate ligands. **L. Sun**, L. Duan, Y. Xu, B. Åkermark

8:45 265. Water oxidation by tris(tetrachlorosemiquinonate)iron(III). **C. G. Pierpont**, P. Nelson, N. Hawkey, J. Kelly, M. Krysiak, H. Huang

9:15 266. Molecular, stable and fast water oxidation catalysts for solar fuel production. **C. L. Hill**

9:45 267. 12-Tungstozincate modified titania electrodes for photoelectrochemical water splitting. **S. K. Pilli**, T. E. Furtak, M. T. Lusk, J. A. Turner, A. M. Herring

10:05 Intermission.

Section B

InterContinental San Francisco
InterContinental Ballroom A

Solar Cells and Solar Fuels

Catalyst: Fuel Production

H. Jia, Y. Lu, L. Sun, and D. Wang, *Organizers, Presiding*

10:15 268. Redox catalysis for solar fuel generation. **E. Fujita**, J. T. Muckerman

10:45 269. Preparation and reactions of hydrogenase models containing a carboxylate function. **B. Åkermark**, L. Sun, W. Gao, T. Åkermark

11:15 270. Modular approach to molecular electrocatalysts for H_2 production and oxidation. **D. L. DuBois**, M. C. R. DuBois, R. M. Bullock

11:45 271. Visible-light-induced highly-selective CO_2 reduction utilizing a p-type semiconductor and the ruthenium complex. **S. Sato**, S. Saeki, T. Morikawa, T. Kajino, T. Motohiro

12:05 272. Titania thin films with red-shifted photoresponse: Non-stoichiometry and cation doping. **P. A. DeSario**, L. Chen, M. E. Graham, K. A. Gray

Section C

InterContinental San Francisco
Grand Ballroom B

Theory and Simulation in Energy Production and Utilization

Cosponsored by PHYS
Q. Ge and J.-G. Wang, *Organizers, Presiding*

8:30 273. Iterative hybrid scheme for accurate and efficient geometry optimization: An extended ONIOM method. W. Guo, A. Wu, Y. Zhang, J. Wu, **X. Xu**

9:15 274. Computational and experimental study of functionalized amidine-based CO2 sorbents. **J. R. Kitchin**, R. Alesi, A. Lee

10:00 275. Size-dependent Al nanoparticle oxidation enthalpy. **S. W. Chung**, S. W. Buckner, P. A. Jelliss, C. E. Bunker, E. A. Guliants

10:20 Intermission.

10:30 276. DFT study of the modulation of bonding between noble metal clusters and CNTs. **J.-G. Wang**

10:50 277. Electronic and structural effects on subnanometer metal catalysis. **J. P. Greeley**, D. Torres-Rangel

11:35 278. Molecular simulation and density function theory for the CO2 Capture in porous materials. **H. Liu**, S. Zhuo, Y. Zhu, Y. Liu, Y. Huang, J. Hu, J. Jiang

Section D

InterContinental San Francisco
Telegraph Hill

CO_2 Capture, Conversion and Utilization

CO_2 Sequestration, Capture, Adsorption, Separation and Management

B.-L. Su and V. Lin, *Organizers, Presiding*

8:35 279. Development and rapid deployment of advanced carbon management technologies. **A. Cugini**, M. Syamlal, B. Morreale

9:10 280. Molecular perspective for CO_2 storage and capture in nanoporous adsorbents and polymeric membranes. **J. Jiang**

9:35 281. Membrane stripping: Desorption of carbon dioxide from aqueous alkali solvents. **M. A. Simioni**, S. E. Kentish, G. W. Stevens

10:00 282. Novel aminosilicone solvents for CO_2 capture. **R. J. Perry**

10:20 Intermission.

10:30 283. Simultaneous desulfurization and CO_2-capture in chemical-looping combustion of sulfur-contaminated synthesis gas. **R. D. Solunke**, G. Veser

10:50 284. Comparison of delaminated zeolite ITQ-6 and SBA-15 for the adsorption of carbon dioxide. A. Zukal, I. Dominguez, J. Mayerova, **J. Cejka**

11:10 285. MUSTANG: A multiple space and time scale approach for the quantification of deep saline formations for CO_2 storage. **G. Wiegand**, A. Niemi, P. Gouze, M. Sauter

11:30 286. Adsorption of carbon dioxide by alkali metal based solids. **B.-T. Zhang**, M. Fan

11:50 287. Oxidation inhibitors for aqueous amines solutions used in a post-combustion CO_2 capture process. **B. Delfort**, P. L. Carrette, L. Bonnard

Section E

InterContinental San Francisco
InterContinental Ballroom B

Hydrogen Storage

Hydride Materials

Y. Hu, *Organizer*
T. Gennett, *Organizer, Presiding*

8:30 288. Combining first principles and thermodynamic calculations to predict evolution of impurity gases from metal hydrides. **M. Allendorf**, V. Stavila, K. C. Kim, D. S. Sholl

9:00 289. Elastic strain energy, thermodynamics, and kinetics of hydride formation in Mg-based thin films. **C.-J. Chung**, S. T. Kelly, E. Senses, B. M. Clemens

9:20 290. Large-scale screening of metal hydrides for hydrogen storage based on equilibrium reaction thermodynamics. **D. S. Sholl**, K. C. Kim, A. Kulkarni, J. K. Johnson

9:40 291. Self-assembled highly-ordered nanoporous hard carbon scaffolds for improved $LiBH_4$ hydrogen sorption. **E. Majzoub**, X. Liu, D. Peaslee

10:00 Intermission.

10:10 292. Tuning the thermodynamics of nanosized metal-hydrides for hydrogen storage applications. **A. Baldi**, M. Gonzalez-Silveira, V. Palmisano, B. Dam, R. Griessen

10:30 293. Magnesium hydride formation studied by low-energy electron microscopy. T. Herranz, K. F. McCarty, B. Santos, **J. de la Figuera**

10:50 294. H_2 sorption properties of carbon supported Mg(Ni) nanocrystallites. **S. S. V. Tatiparti**, R. Bogerd, K. P. de Jong, P. E. de Jongh

11:10 295. Effects of different Ti-compounds on the reversibility of $NaAlH_4$. **P. Rangsunvigit**, Y. Suttisawat, B. Kitiyanan, S. Kulprathipanja

Advances in Fischer-Tropsch Catalysis and Processing

Sponsored by PETR, Cosponsored by CATL (probationary) and FUEL

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Robert J. Madix

From Surface Science to Heterogeneous Catalysis: Fundamental Studies of Reactions on Metal Surfaces

Sponsored by CATL (probationary), Cosponsored by COLL, FUEL and PETR

Catalysis for Sustainability

Catalyst for Biorenewable Energy Applications

Sponsored by CATL (probationary), Cosponsored by AGFD, AGRO, BIOL, BIOT, FUEL and PETR

WEDNESDAY AFTERNOON

Section A

InterContinental San Francisco
Grand Ballroom A

Advances in Coal Conversion Chemistry

Synthesis of Carbons from Coal

A. Chaffee, K. Miura, and J. Qiu, *Organizers*
S. Eser, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 296. Template synthesis of carbon nanofibers/carbon foam composite from coal liquefaction residue. N. Xiao, Y. Zhou, **J. Qiu**

2:05 297. Synthesis of coal-based double walled carbon nanotubes by arc discharge. L. Sun, B. Cai, C. Wang, Z. Zhao, C. Yu, **J. Qiu**, P. Bai

2:25 298. Synthesis of carbon belts from coal via arc-plasma in acetylene. Z. Li, Q. Dong, C. Hu, **J. Qiu**

2:45 299. Towards the synthesis of nuclear graphite from co-cokes and anthracites. **M. S. Nyathi**, C. Burgess Clifford, H. H. Schobert

3:05 Intermission.

Section A

InterContinental San Francisco
Grand Ballroom A

Advances in Coal Conversion Chemistry

Coal Dissolution and Conversion Products

S. Eser, and J. Qiu, *Organizers*
A. Chaffee, and K. Miura, *Organizers, Presiding*

3:15 300. Dissolution and dispersion of coal in ionic liquids. **P. C. Painter**, N. Pulati, R. Cetiner, M. Sobkowiak, G. Mitchell, J. Mathews

3:35 301. Desulfurization of coal extract by metal loaded carbon. **Y. Mochizuki**, K. Sugawara

3:55 302. Solvent extraction of coal to produce feedstocks for a laboratory scale coker. **C. E. Burgess**, J. Griffith, V. Karri, M. Achimugu

4:15 303. Inorganic constituents of coal liquefaction. **S. A. Luchner**, S. F. Miller, B. G. Miller

4:35 304. Total analyses of a Kentucky coal: Proton NMR by variable cycle time CRAMPS, ^{13}C NMR by CPMAS, As, Be, Hg, Pb and U by ICPMS. **B. C. Gerstein**, C. Ebert, X. Hsu

4:55 305. Rheological properties of coal ash slag at high temperatures. **S. Wenjia**, S. Yimin, Z. Zibin, K. Shuntarou

Section B

InterContinental San Francisco
InterContinental Ballroom A

Solar Cells and Solar Fuels

Hydrogen Production

Y. Lu, *Organizer*
Y. Song, *Presiding*
H. Jia, L. Sun, and D. Wang, *Organizers, Presiding*

1:30 306. Hydrogen production from overall water splitting on oxynitride photocatalysts. **J. Kubota**, K. Domen

2:00 307. Dye-sensitized semiconductor photoelectrochemical cells for overall water splitting. **S.-H.A. Lee**, W. J. Youngblood, L. K. Blasdel, T. E. Mallouk, T. A. Moore, A. L. Moore, D. Gust

2:20 308. Nanostructured titania thin films for H_2 production by water photoelectrolysis and photoreforming of renewable sources in PEC solar cells. **G. Centi**, S. Perathoner, R. Passalaacqua, C. Ampelli

2:40 309. Direct synthesis of capped platinized TiO_2 nanoparticles for subsequent sensitization by donor-chromophore-acceptors: Towards hydrogen generation from water. **D. C. Johnson**, M. S. Lazorski, H. Jia, C. M. Elliott, A. L. Prieto

3:00 Intermission.

Section B

InterContinental San Francisco
InterContinental Ballroom A

Solar Cells and Solar Fuels

Hydrogen Production

Cosponsored by CATL (probationary)
Y. Lu, *Organizer*
W. Zhou, *Presiding*
H. Jia, L. Sun, and D. Wang, *Organizers, Presiding*

3:10 310. Light enhanced CO_2 reduction using porphyrin nanofiber-decorated electrodes. **Y. Song**, R. M. Garcia, L. Evans, J. E. Miller, J. A. Shelnutt

3:30 311. Nanostructured MoS_2 for solar hydrogen production. **Z. Chen**, S.-J. Choi, J. Kibsgaard, T. F. Jaramillo

3:50 312. Photocatalytic hydrogen evolution by tungsten oxide dispersed in mesoporous MCM-48. **D. Zhao**, A. Rodriguez, R. T. Koodali

4:10 313. Thiophenylation and secondary reactivity at low defect density Si(111) surfaces for covalent attachment of fuel generating catalysts. **L. E. O'Leary**, E. Johansson, M. J. Rose, B. S. Brunschwig, R. H. Grubbs, N. S. Lewis

4:30 Concluding Remarks.

Section C

InterContinental San Francisco
Grand Ballroom B

Theory and Simulation in Energy Production and Utilization

Cosponsored by PHYS
Q. Ge and J.-G. Wang, *Organizers, Presiding*

1:30 314. Density functional and slab model studies of the structure of Pd/ZnO catalyst active to methanol steam reforming. Y. Huang, W. Ding, **Z.-X. Chen**

2:15 315. Atomic arrangement and catalytic activity of Au-Pt and Au-Pd alloy surfaces: A combined quantum mechanical and Monte Carlo study. **G. S. Hwang**

3:00 316. Comparative study of CO2 interaction with the transition metal dimers. **Q. Ge**, J. Tyrrell, J. Ye, C. Liu

3:20 Intermission.

3:30 317. Quantifying the effects of surface coverage on the rates of catalytic oxidations. **W. F. Schneider**

4:15 318. Reaction mechanism of phenol alkylation with tert-butyl alcohol over Hβ zeolite: An ONIOM study. **X. Nie**, X. Liu, C. Song, M. Liu, X. Guo

4:35 319. Low-temperature oxidation of hydrocarbon fuels in a motored engine. **P. L. Perez**, A. L. Boehman

4:55 320. Comparison of the performance of synthetic liquid fuel processes. **A. C. Beath**

Section D

InterContinental San Francisco
Telegraph Hill

CO_2 Capture, Conversion and Utilization

CO_2 Sequestration, Capture, Adsorption, Separation and Management

V. S.-Y. Lin, and B.-L. Su, *Organizers*
J. Cejka, *Presiding*

1:30 321. Design and synthesis of porous materials toward gas capture. **G. Zhu**

1:55 322. Use of $Cu_3(BTC)_2$ metal-organic framework as sorbent for gas separations: Study of CO_2/CH_4 separation for PSA applications. **L. Hamon**, E. Jolimaître, G. Pirngruber

2:15 323. Novel custom gas sorption analyser for the assessment of adsorbents for CO2 capture by vacuum swing adsorption. G. P. Knowles, Z. Liang, P. A. Webley, **A. L. Chaffee**

2:35 324. Mobile NIR inline monitoring device for processes with CO_2. **G. Wiegand**, S. Johnsen, B. Zehnder

2:55 Intermission.

3:05 325. Ionic liquids for post-combustion CO_2 capture: Tunable capacities and enthalpies. B. F. Goodrich, L. E. Ficke, **J. F. Brennecke**

3:30 326. Ceramic sorbents for production of oxygen-enriched carbon dioxide stream. Z. Rui, J. Ding, Y. S. Lin, **Y. Li**

3:50 327. Reversible acid gas capture using CO2-binding organic liquids. **D. J. Heldebrant**, P. K. Koech, C. R. Yonker, J. Rainbolt, F. Zheng

4:10 328. Capturing of CO_2 from flue gases over MgO/Al_2O_3 sorbent in fluidized bed. L. Li, W. Peng, F. Wang, N. Zhao, F. Xiao, N. Wang, X. Liu, **W. Wei**, **Y. Sun**

4:30 329. Mg modified mesoporous material SBA-15s and their CO_2 adsorpotion capacities. H. Zhao, C. Jing, J. Zhou, J. Hu, **H. Liu**

4:50 330. Introducing mechanical action in liquid cleaning processes with carbon dioxide by clathrates. A. Hebach, A. Oberhof, N. Dahmen, **G. Wiegand**

Section E

InterContinental San Francisco
InterContinental Ballroom B

Hydrogen Storage

Carbon Based Materials

Cosponsored by CATL (probationary)
Y. Hu, *Organizer*
C. Engtrakul, *Presiding*
T. Gennett, *Organizer, Presiding*

1:30 331. Electric charge and hydrogen storage. **J.-Y. Hwang**, S. Shi, X. Sun

2:00 332. High hydrogen sorption in covalently linked carbon nanotube scaffold -a theoretical investigation. **M. Mani Biswas**, T. Cagin

2:20 333. Investigation of spillover mechanism for hydrogen storage in transition metal doped single wall carbon nanotubes by 4-probe conductivity and FTIR spectroscopic studies. **R. Bhowmick**, B. M. Clemens

2:40 Intermission.

2:50 334. Measuring hydrogen adsorption on high surface area samples: Avoiding calibration errors. **P. A. Parilla**, K. O'Neill, R. Knott, T. Gennett, J. L. Blackburn, C. Engtrakul, J. Bult, L. J. Simpson

3:20 335. Hydrogen spillover on ruthenium-decorated carbon based substrates. **T. Gennett**, K. J. O'Neill, J. B. Bult, T. Baumann, J. Liu, L. Simpson

3:40 336. Hydrogen storage properties of nanostructured graphite-based materials. **Y. Zhang**, D. Book, D. Reed, V. Mann

4:00 Concluding Remarks.

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Peter C. Stair

From Surface Science to Heterogeneous Catalysis: Fundamental Studies of Reactions on Metal Surfaces

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Catalysis for Sustainability

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Catalysis for Sustainability

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THURSDAY MORNING

Section A

InterContinental San Francisco
Union Square

Green Chemistry on Fuels of the Future

Alternative Processes

W.-L. Jang, *Organizer*
M. Shirai, and J. Spivey, *Presiding*

8:30 337. Feasibility of gas-expanded lubricants for increased energy efficiency in power turbines. S. Wang, **A. F. Clarens**

8:50 338. Selective oxidation of ethylene in a model “dirty” synthesis gas stream: An experimental and kinetic modeling study. **S. M. Villano**, J. Hoffmann, H.-H. Carstensen, A. M. Dean

9:10 339. Chemical processes using supported metal catalysts and supercritical fluid. **M. Shirai**, N. Hiyoshi, A. Yamaguchi, O. Sato

9:30 340. Oxy-CO_2 reforming of methane on PdNi/Y_2O_3: Role of synthesized supports on Pd-Ni interaction. U. Oemar, K. Hidajat, **S. Kawi**

9:50 Intermission.

10:00 341. Synthesis of higher oxygenates from syngas: Challenges for catalyst selectivity and activity. **J. J. Spivey**, N. Kumar

10:45 342. Novel photobioreactors based on microalgae immobilized in silica gels obtained by "Chimie douce" for biofuel production. **A. Leonard**, J. Rooke, H. Sarmento, J.-P. Descy, B.-L. Su

11:05 343. Hydrothermal conversion of water hyacinth (*Eichhornia crassipes*) to bio-oil. L. Zhang, D. Zhou, **S. Zhang**, **J. Chen**

11:25 344. Advances in the feedstocks, processes, reactors and catalysts for producing biodiesel. **F. Shubo**, Z. Bingzhu, Z. Erli

11:45 Concluding Remarks.

Section B

InterContinental San Francisco
Grand Ballroom C

Solar Cells and Solar Fuels

Inorganic, Thin Film PV

H. Jia, Y. Lu, L. Sun, and D. Wang, *Organizers, Presiding*

8:30 345. Novel synthetic routes to p-type semiconductor absorbers for thin film heterojunction solar cells. **D. R. Radu**

8:50 346. Amorphous silicon nanodome solar cells with efficient light harvesting. **J. Zhu**, C. M. Hsu, Z. Yu, S. Fan, Y. Cui

9:10 347. Deposition of ZnS and CdS for graded CIGS buffer layers using in situ production of H_2S. **J. R. Bakke**, S. F. Bent

9:30 348. Fabrication of low-cost $CuInS_2$ solar cells by Air-stable Ink Rolling (AIR) process. **S. T. Connor**, B. Weil, Y. Cui

9:50 349. Cu(In,Ga)Se_2 (CIGS) nanocrystal "Inks" for solution-processable photovoltaics. **M. G. Panthani**, V. A. Akhavan, B. W. Goodfellow, B. A. Korgel

10:10 Intermission.

InterContinental San Francisco
Grand Ballroom C

Solar Cells and Solar Fuels

Nanostructure for Enhanced Efficiency

H. Jia, Y. Lu, L. Sun, and D. Wang, *Organizers, Presiding*

10:20 350. Single molecule studies of electronic coupling in semiconductor nanocrystal clusters. **A. Van Orden**, D. Shepherd, K. Whitcomb, M. Gelfand, P. M. Goodwin

10:50 351. Ab initio mechanism for singlet fission in acene solar cells through dark states. **P. M. Zimmerman**, Z. Zhang, C. B. Musgrave

11:10 352. Synthesis of Type II 3D coaxial nanocable arrays for photovoltaic device fabrication. K. Wang, J. Chen, Z. Zeng, **W. Zhou**, Y. Zhang, J. Pern, Y. Yan, A. Mascarenhas

11:30 353. Improving light absorption in thin silicon nanowire photovoltaics. **E. C. Garnett**, C. Peters, M. Brongersma, Y. Cui, M. McGehee

12:00 354. Design and synthesis of $CuInS_2$-based nanostructured materials towards solar cell applications. **X. Wang**, Y. Lu

Section C

InterContinental San Francisco
Grand Ballroom B

Theory and Simulation in Energy Production and Utilization

Q. Ge and J.-G Wang, *Organizers, Presiding*

8:30 355. Insights in the transformation of oxygenated hydrocarbons at metal catalysts from DFT and scaling relations. **P. Sautet**

9:15 356. Ethanol synthesis and decomposition on Rh. **P. Liu**, Y. M. Choi

10:00 357. Building complex kinetics models with INGen. C. A. Bennett, Z. Hou, C.-J. Kim, B. M. Moreno, **M. T. Klein**

10:20 358. Mechanism and energetics of glucose conversion to hydromethylfurfural. Y. Cao, H. Dong, J.-L. Li, M. Nimlos, **X. Qian**

10:40 Concluding Remarks.

Section D

InterContinental San Francisco
Grand Ballroom A

CO_2 Capture, Conversion and Utilization

Bioconversion, Photosynthesis and Biocapture

V. S.-Y. Lin, *Organizer*
B.-L. Su, *Organizer, Presiding*

8:30 359. Sunlight storage: From dyads to tetrads and charge separation. **A. C. Benniston**

9:05 360. Methanol synthesis from carbon dioxide based on the artificial photosynthesis and dehydrogenases. **Y. Amao**

9:30 361. Artificial inorganic leafs inspired by natural photosynthesis. **T. Fan**, H. Zhou, D. Zhang

9:55 362. Bioconversion of CO_2 by photochemical materials. **C. F. Meunier**, P. Van Cutsem, Y.-U. Kwon, B.-L. Su

10:15 Intermission.

10:25 363. Photosynthetic efficiency in production of microalgae. **O. Pulz**

11:00 364. Exploiting photosynthesis: Designing novel bioreactors by the symbiosis of living picoplankton and abiotic silica gel. **J. C. Rooke**, A. Léonard, H. Sarmento, J.-P. Descy, B.-L. Su

11:20 365. Chitosan for separation and capture of CO2 from flue gas. **T. G. Levitskaia**, A. J. Casella, J. M. Peterson

11:40 366. CO_2 selective catalytic photoreduction on Pt/TiO_2 nanotube for renewable energy. **Q.-H. Zhang**, W.-D. Han, Y.-J. Hong, J.-G. Yu

12:00 Concluding Remarks.

Section E

InterContinental San Francisco
InterContinental Ballroom B

Advances in Coal Conversion Chemistry

Coal Gasification and Liquefaction

A. Chaffee, S. Eser, and K. Miura, *Organizers*
J. Qiu, *Organizer, Presiding*

8:30 367. Advanced separation engineering of coal by Organo-refining for adding value. **D. K. Sharma**

8:50 368. Measurement of CO_2 gasification rate of upgraded coal char using a mini direct heating reactor at high temperature and high pressure. M. Makino, R. Ashida, **K. Miura**

9:20 369. CO_2 gasification rate analysis and modeling under high CO_2 partial pressure conditions. **H. Watanabe**, S. Umemoto, S. Kajitani, S. Hara, H. Makino

9:40 370. Liquefaction of a series of high volatile bituminous coals recovered over a 300m depth interval. **A. L. Chaffee**, G. Lay, M. Marshall, W. R. Jackson, Y. Fei, T. V. Verheyen, P. J. Cassidy, S. G. Scott

10:00 Intermission.

10:10 371. Detailed characterization of coal-derived liquids from direct coal liquefaction on supported catalysts. **J. Stihle**, C. Geantet, D. Uzio, N. Charon

10:30 372. Integrated process of coal pyrolysis with methane activation by dielectric barrier discharge plasma. X. He, L. Jin, Y. Zhao, **H. Hu**

10:50 373. Effect of coal extract on coke strength and pore structure. **K. Koyano**, K. Ueoka, T. Takanohashi, T. Shishido, N. Okuyama, N. Komatsu

11:10 Concluding Remarks.

Catalysis for Sustainability

Catalyst for Biorenewable Energy Applications

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Catalysis for Sustainability

Electrocatalyst for Fuel Cells

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THURSDAY AFTERNOON

Catalysis for Sustainability

Catalyst for Biorenewable Energy Applications

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Catalysis for Sustainability

Electrocatalyst for Fuel Cells

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