SUNDAY MORNING

Section A

Hilton Grand Ballroom B

General Papers in Fuel and Energy Chemistry

A. M. Herring, Organizer, Presiding

8:00 Introductory Remarks.
8:05 1. New theory for basic water structure and potential fuel and energy applications. R. E. Winars, Organizer
8:30 2. Cyclic-Cycle: Carbon dioxide capture, activation and product release. P. Styzing, O. Asachenbrenner, S. Supapholme
8:55 3. Enhance of surfactant on the dioxygenase biosurfacta. H. Chen, W. Li
9:45 5. Application of computational chemis to combustion processes: Generation of reliable thermodynamic data for the aro matics oxidation mechanisms. F. Louis, S. Canneux, M. Ribaucour, A. El Bakal, J. P. Pauwel
10:10 Intermission.
10:30 6. Exploring the chemical reactivity of asphaltene. M. N. Siddiqui
11:45 9. Systematic exploration of hydrogen atom transfer sites in alkyl, and func tionalized radicals, as predicted by com puter ab initio methods. C. J. Hayes, D. R. Buresh Jr.
12:10 Concluding Remarks.

Section B

Hilton Grand Ballroom A

Alternative Hydrocarbons: Tar Sands, Oil Shale, and Heavy Oil Production, Processing, and Chemistry Cosponsored by PETF

S. Eser, E. M. Stauberg, J. F. Schabron, and P. Rahimi, Organizers

8:15 Introductory Remarks.
10:00 Intermmission.
10:20 Introductory Remarks.
12:05 Concluding Remarks.

SUNDAY AFTERNOON

Section A

Hilton Grand Ballroom B

General Papers in Fuel and Energy Applications

A. M. Herring, Organizer, Presiding

A. M. Dean and H. H. Cartensen, Presiding

2:00 Introductory Remarks.
2:20 1. Substantial enantioselective ethanol by 2012: NREL’s thermochemical platform. E. J. Frederick
2:30 2. Biomass characterization and organosolv pretreatment of Buddleja davidii. B. B. Hallane, P. Sannirgh, V. Pu. May, R. Murphy, A. J. Ragwasus
3:45 Intermission.
3:45 5. Development of low temperature glycerol and ethylene glycol fuels cells capable of high energy density and com plete oxidation. R. L. Arechedia, S. D. Minter
5:45 Concluding Remarks.

Section B

Hilton Grand Ballroom A

Gas Hydrates and Clathrates

Hidrogenate Nature

C. A. Koh, E. D. Stican, and A. K. Sum, Organizers

Puppel and J. A. Ripmeester, Presiding

8:00 Introductory Remarks.
8:05 41. Energy and hydrates: An overview inside the fossilise and in nature. E. D. Sloan
8:45 42. Japan’s national gas hydrate pro gram. M. Kurishia
9:25 43. India’s national gas hydrate pro gram. V. Sibal
10:00 Intermission.
10:25 44. China’s national gas hydrate program. S. Fan
11:05 45. Overview of energy-related studies of gas hydrate in Canada. S. R. Dallimore
12:25 Concluding Remarks.

Section C

Hilton Topaz Room

Methods and Techniques in Analytical Characterization for Fuel Nanoscience Cosponsored by NANO

R. E. Winars, Organizer

R. J. Pugmire, Organizer, Presiding

8:30 Introductory Remarks.
8:35 47. Applications of pair distribution function analysis to study energy-related materials. K. H. Chapman, P. J. Chupas, R. E. Winars, R. J. Pugmire
9:00 48. In situ NMR and pair distribution function studies of local structure in silicon anodes for lithium ion batteries. B. Kay, R. Bhattacharya, C. P. Grey
10:00 51. In situ characterization of hetero peneous catalysis using time-resolved X-ray diffraction. J. C. Hanson, X. Wang, W. Lin, L. Barro, G. Zhou, M. Esritza, J. A. Rodriquez

Nanotechnology in Catalysis VI Sponsored by CATL (probaton). Cosponsored by CCLL, FUEL, & IEC, PETR, and NANO

MIXDAY AFTERNOON

Section A

Hilton Grand Ballroom B

Catalytic Upgrading of Fuels Cosponsored by ACCI

C. K. Nanula, Organizer

S. H. Overbury, Organizer, Presiding

2:00 Introductory Remarks.
2:24 55. Catalytic upgrading of Fischer-Tropsch syncrude to fuels. A. De Klerk, R. Nel
3:05 56. Overview of Fischer-Tropsch aque ous product refining strategies. A. De Klerk, R. Nel
4:15 Intermission.

The official technical program for the 23th National Meeting is available online at oasys2.confex.com/acs/237nm/ techprogram/
In situ FT-IR studies of CO and CO₂ hydrogenation for stack supported Rh and Rh-Li catalysts. V. Schwartz, K. More, S. H. Overbury, A. Ebgebi, J. J. Spivey
5:35 61. Effect of CO₂ on CO hydrogenation to ethanol over Rh-Mn-Li/TiO₂ versus Rh-Mn-Fe/TiO₂. A. Ebgebi, J. J. Spivey
6:00 Concluding Remarks.

Section B

Hilton Grand Ballroom A

Gas Hydration and Clathrates
Hydrates in Nature

C. A. Koh, and A. K. Sum, Organizers
S. R. Dalimore, Presiding
E. D. Sloan, Organizer, Presiding

2:00 Introductory Remarks.

2:10 62. Methane hydrates and global climate change: A status report. C. Ruppel
3:15 64. Gas production from methane hydrates. M. J. Castaldi, Y. Zhou, J.-Y. Eulpale
3:40 Intermission.

5:15 Discussion.

Section C

Hilton Topaz Room

Methods and Techniques in Analytical Characterization of Fuel Nanocatalysts Co-sponsored by NANO

R. J. Pugmire, Organizer
R. E. Winans, Organizer, Presiding

2:00 Introductory Remarks.

2:05 68. Interaction of CO₂ with coal via SANS. J. M. Calo, E. J. Bain
2:10 69. Raman, S. Settelf, A. H. Clemens
2:50 69. S-XANES analysis of sulfur forms in coals and kerogen. T. B. Bolin
3:20 69. Mass spectrometry of CO₂ in the presence of bentonite particles. R. P. Warpinski
3:40 Intermission.

3:40 71. Mass spectral characterization of a VSC. M. T. Cheng, J. D. Hudson, C. DeMagallie
4:05 72. An improved method for determination of inorganic parameters from constant heating rate TGA of shale pyrolysis data. J. L. Hillier, J. S. Fletcher, G. Isaacson, J. Ortig, T. H. Fletcher
4:30 73. Fluorocarbon molecular frameworks. C. Yang, M. A. Omari
4:55 74. Electrochemical hydrogenation and hydrogen evolution on carbon nanotubes. Z. Zhang, P. Zhang, C. B. Musgrave
5:20 Concluding Remarks.

Techno-Fuel

Section D

Hilton Grand Ballroom C

Catalysis and Reactors

General Papers in Fuel and Energy Chemistry

A. M. Herrera, Organizer
1:30–4:00
76. Facile enrichment of tocopherols by automated flash chromatography. J. E. Silver, N. Fowler, P. Bellinghausen, C. Scanton
77. Novel catalysts for transesterification of vegetable oils. V. A. Curtis-Palmer, M. W. Majewski
78. Polyporex and platinum nanoparticulate for fuel cell applications. X. Zhang, F. N. Crespo, V. Zucolotto, S. K. Manhart, L. H. C. Mattoso, K. Bergamaschi
79. Ionic liquids as “green” replacements for hydrocarbons in benzhydryl resol polymerization. M. S. Rosander, S. Schneider, T. W. Hawkins
82. Withdraw
83. Study on the effects of activator on the stabilisation of sulphated cobalt phthalocyanine in alkaline solution. X. Li, D. Xia, Y. Xiang
85. Enzymatic biocatalyst for butanol production. S. Bhac, S. Diner
87. Factors affecting lignin measurements in dilute acid pretreated herbaceous feedstock. L. Katarina, D. W. Templeton, D. J. Schell, M. F. Davis
88. Immobilization of the first five glycolyzed enzymes for biocatalytic applications. C. E. Menis, S. Diner
89. Methanol-based catalyst based on NAD-dependent enzymes immobilized at electrode by hydrophobically modified Nanol. P. K. Addeo, S. Diner
90. Optimization of PQQ-dependent alcohol dehydrogenase activity in Gluconobacter sp. 33 for use in biocatalytic processes. C. E. Menis, S. Diner
91. Performance of PEG membranes in scale-up for pervaporation of gas desalination. L. Lin
92. Polyarylene ether's carrying pendant (3-sulfonatedpheny) sulfonyl groups. M. Abdalst, D. R. Douglass, E. Fossam
93. Producing energy efficient concrete using coal fly ash. M. Ch, S-P. Chou
94. Pyrolysis of lignin model compounds using a hyperthermal nozzle: Decomposition pathways of the any ethers. C. Mukarakate, A. M. Schier, D. J. Robbrough, B. Elston, M. R. Nimlos, M. F. Davis
96. Tar quantification from a fluidized bed biomass gasification: Gas chromatographic and gravimetric methods. H. Cui, S. Q. Tun

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11:35 104. Transition-metal-based catalytic systems for the deoxygenation and metathesis of alkenes: Solution-phase and solid-supported iodine-based precursor cata-
lysts. A. S. Goldman, H. Gu, M. C. Crooksh, Z. Huang, K. Krogh-Jespersen, S. Kundi, L. S. Scott
12:00 Concluding Remarks.

Section B

Hilton Grand Ballroom A

Gas Hydration and Clathrates

Hydrate Flow Assurance & Technology

E. D. Sloan and A. K. Sum, Organizers
M. Kurihara, Presiding
C. A. Koh, Organizer, Presiding

8:00 Introductory Remarks.

9:40 Intermission.

10:00 108. Studies of mass transfer resis-
10:25 109. Enhance rates of gas hydrate formation in a silica sand matrix compared to a stirred vessel. P. Linga, C. Haligva, J. A. Ripmeester, P. Engles
11:00 110. Progress on the gas hydrate processes for production and CO2M separat-
ion using a large scale apparatus. P. Linga, R. Kumar, J. A. Ripmeester, P. Engles
11:40 Discussion.

Section C

Hilton Topaz Room

Emissions from Combustion Processes: Environmental, Issues, Assessment, and Control

J. S. Lightly, G. Silcox, and J. H. Heibe, Organizers

8:00 Introductory Remarks.

8:55 114. Control of fuel gas mercury emis-
sions: Effects of acid gases on sorbent reactivity. E. Olson
9:45 116. Fate of arsenic and selenium in air pollution control devices in coal-fired power plants. C. Senior
10:00 Intermission.

10:55 118. Soot deposit properties in practi-

† Cooperative Co-sponsored
Division of Geochemistry

D. B. Kent, Program Chair

SUNDAY MORNING

Section A
Hilton Alpine Ballroom East

Cocorepition of Metals during Chemically and Biologically Induced Mineral Precipitation

Y. Fujita and A. Kappler, Organizers

8:30 Introductory Remarks.
8:40 1. Adding structure to reactivity: How do aqueous oxides really react? W. H. Casey
9:10 2. Ca, Zn, and Cd ions at buried solid/surface interfaces studied by second harmonic generation. F. M. DeGeer, J. N. Malin, P. L. Hayes
9:50 4. Cocorepition in the barite interstratified family. C. Zhe
10:20 Intermission.
11:10 6. Induced precipitation of apatite as a strategy to reduce Sr mobility in the subsurface. K. E. Wright, Y. Fujita, D. E. Hainey

Section B
Hilton Salon I

Metal and Mollusk Sedimentation and Adsorption in Honor of D. O. Leckie

Surface Complexation Modeling of Mineral Surfaces Co-sponsored by EWP

M. M. Benjamin, W. P. Elia, B. D. Kent, C. Papelli, G. D. Redden, and A. P. Robertson, Organizers

J. A. Davis and K. F. Hayes, Organizers, Presidng

8:30 Introductory Remarks.
8:50 2. Surface complexation: From models systems to the natural oxide fraction. T. Hiemstra, W. H. van Remsrijk
10:10 4. Intermission.
10:50 6. Surface complexation models of ion adsorption in soils. G. Sposito, S. Goldberg

11:15 7. Sorption of trivalent metals on uranium(VI) silicates. S. L. Holbrook
11:35 8. Relative contributions of surface and solution reactions to the acid-base chemistry of gibbsite suspensions. A. K. Karamalidis, D. A. Dzombak

Section C
Hilton Salon II

Molecular Computational Geochemistry for Water-Rock Interactions

B. R. Bickmore and K. M. Rosso, Organizers

8:30 Introductory Remarks.
8:35 1. Computer simulations of the interaction of water with complex mineral surfaces and clusters. N. H. de Leeuw
9:50 4. Structure and transport behavior of nanofractured water and enhanced hydrothermal uranium ion formation. S. H. Garafalini, T. Mahadevan
10:15 Intermission.
10:25 5. Diffusion of water and solutes near clay surfaces. Bridging the nanopore and molecular scales. I. C. Bourg, D. Sposito
10:50 6. Structure and dynamics of water at mineral interfaces and in nanoconfined systems: Connecting molecular modeling with experimental observations. A. G. Katritzky
11:40 8. Potential of mean force studies of the adsorption of rare earth elements to detect rorden quartz. A. Clark, M. C. F. Wander

SUNDAY AFTERNOON

Section A
Hilton Alpine Ballroom East

Cocorepition of Metals during Chemically and Biologically Induced Mineral Precipitation

Y. Fujita and A. Kappler, Organizers

1:30 2. Iron cycling at neutral pH and the production of iron oxyhydroxides with unique morphologies and properties by oxygen-dependent iron-oxidizing bacteria. D. Emerson
3:00 Intermission.

Please refrain from using cellular telephones and cameras during technical sessions.