545. Superior reductive amination with silica-gel bound $^{-}CNBH_3$ (*Si*-CBH). **B. L. Sumbler**, P. N. Grenga, R. Priefer
546. Synthesis of allenes and amines from propargyl boron derivatives. N. A. Petasis, **C. Arden**
547. Synthesis of N, N-di(2-aminoethyl)-1,3-propylenediamine. **X. Zhang**, W. Wu
548. Synthesis of substituted 2,6-dioxabicyclo[3.2.1]octane ring systems using a Payne rearrangement–cascade epoxide opening approach. **R. A. Kowtoniuk**, T. W. Funk
549. Synthesis of vinylfluorides via Julia-Kocienski reaction. G. K. S. Prakash, **A. Shakhmin**, M. Zibinsky, S. Chacko, I. Ledneczki, G. A. Olah
550. Two directional olefinic-ester ring-closing metathesis using reduced Ti alkylidenes: A rapid entry into polycyclic ether skeletons. **Y. Zhang**, J. D. Rainier
551. Utilization of polydimethylsiloxane membranes for the site-isolation and recycling of $PdCl_2$ and one-pot cascade reactions. **A. L. Miller II**, N. B. Bowden
552. Vanadium-catalyzed oxidative bromination reaction under atmospheric oxygen. **K. Kikushima**, T. Moriuchi, T. Hirao
553. $P(PhCH_2NCH_2CH_2)_3N$: A highly effective Lewis-base catalyst for Mukaiyama aldol reactions of aliphatic, aromatic and heterocyclic aldehydes, and a trifluoromethyl ketone. **V. R. Chintareddy**, K. Wadhwa, J. G. Verkade
554. Palladium catalyzed intermolecular hydroamination of η-protected anilines with π-electron-rich vinyl ethers. **N. K. Pahadi**, J. A. Tunge
555. Palladium-catalyzed oxidative difunctionalization of terminal alkenes using organostannanes. **K. B. Urkalan**, **M. S. Sigman**
556. Pd-catalyzed hydroarylation of terminal 1,3-dienes. **L. Liao**, M. S. Sigman
557. Pd-catalyzed hydrofunctionalizations of styrenes and dienes. **S. M. Podhajsky**, K. M. Gligorich, S. A. Cummings, Y. Iwai, M. S. Sigman
558. A direct and practical synthesis of phenyl esters from phenol and carboxylic acids under clean chemistry conditions. **K. Mukkanti**, K. Kankanala, V. R. Reddy, S. Pal
559. A "one-pot" process for the preparation of trans-n-benzyl-3-hydroxy-4-hydroxymethylpyrrolidine. **P. Zhang**, M. Cedilote, T. P. Cleary
560. Bouveault-Blanc reduction using stabilized alkali metals: An alternative method for ester reduction. **B. S. Bodnar**, P. F. Vogt
561. Convergent epoxide based approaches for the synthesis of the C15–C25 bafilomycin A1 polypropionate chain. **E. M. Valentín-Nevárez**, M. Mulero, K. Rosa-Pérez, J. A. Prieto
562. Copper-promoted diastereoselective intramolecular aminooxygenation of alkenes. **M. C. Paderes**, S. R. Chemler
563. Diastereoselective reductive aminations of α-fluoroketones. **W. R. Hess**, J. Janke, T. A. Davis
564. Dihydropyran formation by a two step process. **Z. Wright**, **L. McNulty**
565. Divergent reactivity in tandem reduction-Michael ring closures of five- and six-membered cyclic enones. **R. A. Bunce**, B. Nammalwar
566. Enantioselective palladium-catalyzed difunctionalization of alkenes containing an o-phenol. **K. H. Jensen**, T. P. Pathak, M. S. Sigman
567. Epoxide based approach for the elaboration of a syn,anti,syn precursor fragment for the synthesis of the scytophycin c polypropionate chain. **J. Rentas-Torres**, J. A. Prieto
568. Expanding the scope of sulfonium ylide [3,3] sigmatropic rearrangements. **V. V. Boyarskikh**, G. Glover, A. Nyong, J. D. Rainier
569. Extending the scope of the tethered aminohydroxylation. **C. K. A. Callens**, T. J. Donohoe
570. Flow chemistry methods for the synthesis chemokine receptor ligands. **T. P. Petersen**, A. Ritzén, T. Ulven
571. Highly efficient selective monohydrolysis of dialkyl malonates. **S. Niwayama**, H. Cho
572. Hydrogen gas-free Pd/C-catalyzed PCB degradation. **S. Ishihara**, A. Ido, T. Maegawa, Y. Monguchi, S. Wada, H. Nagase, H. Sajiki
573. Hypervalent iodine compounds as oxidants in phthalocyanine catalyzed oxidations of anthracene. **I. M. Geraskin**, O. Pavlova, V. N. Nemykin, V. V. Zhdankin
574. Isolation, handling, and properties of neat allylic fluorides. **E. Lee**, D. V. Yandulov
575. Methods for the preparation of 2-arylvinyl methyl ethers. **K. R. Davis**, D. A. Hunt
576. Microwave-assisted aza-Cope rearrangement—Mannich cyclization of conformationally mobile amino alcohols: Challenges in the stereoselective synthesis of acylpyrrolidines. **A. M. Kaufmann**, H. A. Lindsay
577. Microwave-assisted deprotection of Boc-protected amines and amino acid derivatives using solid phase supported sulfonic acids in a catch-release manner. R. Lundin, **P. Ioannidis**, M. Östbye
578. Modularly designed organocatalytic assemblies for nitro-Michael addition reactions. T. Mandal, S. Muramulla, **C-G. Zhao**
579. N-heterocycle carbenes (NHC) as organocatalysts in biodiesel synthesis. H. Palencia, **C. Ritchie**
580. New applications of the allylic diazene rearrangement. **M. L. Shrestha**, W. Qi, M. C. McIntosh
581. New method for synthesis of fluorinated α-aminophosphonates with gallium triflate as catalyst. G. K. S. Prakash, **R. Ismail**, M. Zibinsky, T. Mathew
582. Olefinic-lactone cyclizations to macrocycles. **J. Rohanna**, J. D. Rainier
583. One-pot, unsymmetric Cadiot-Chodkiewicz reaction utilizing an in situ ethynylsilane deprotection. **L. R. Cullen**, J. C. Furgal, J. B. Gianino, A. M. Hamlin, J. W. Lezotte, M. J. Mio
584. Organocatalytic asymmetric synthesis of α-hydroxyphosphinates. **C-G. Zhao**, S. Samanta, S. Perera
585. Orthogonal silane protecting group methods for modified Sonogashira couplings. **G. M. Ambrosi**, M. L. Bugeja, D. J. Dumais, S. Martinez, A. Ward, M. J. Mio

PETR

Division of Petroleum Chemistry

K. Fjare, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Alternative Hydrocarbons: Tar Sands, Oil Shale, and Heavy Oil: Production, Processing, and Chemistry (see *FUEL*, Sun)

Catalysis for Cellulosic Feedstock Conversion (see *CATL (probationary)*, Mon)

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend (see *CATL (probationary)*, Tue, Wed)

Nanotechnology in Catalysis VI (see *CATL (probationary)*, Sun, Mon, Tue, Wed)

SOCIAL EVENTS:
Joint PETR/FUEL Dinner: Tue
Symposium Organizer Breakfast: Mon

BUSINESS MEETINGS:
Business Meeting: Tue
Executive Committee Meeting: Sat
Program Committee Meeting: Sat

SUNDAY MORNING

Section A

Hilton
Salon III

Refining and Petrochemicals Using Renewable Feedstocks
Transforming Oil Refining into Biorefining
Cosponsored by CATL (probationary)

B. H. Shanks, K. Fjare, and C. Zhang, *Organizers*

10:00 Introductory Remarks.
10:10 **1.** Catalytic activation and conversion of biomass. **P. O'Connor**
11:00 Intermission.
11:15 **2.** Biogasoline production from catalytic cracking of vegetable oil in a biorefinery. **S. Bhatia**, Y. K. Ong
11:40 **3.** Next generation hydrocarbon biorefineries. **J. R. Regalbuto**

Alternative Hydrocarbons: Tar Sands, Oil Shale, and Heavy Oil: Production, Processing, and Chemistry Sponsored by FUEL, Cosponsored by PETR‡

SUNDAY AFTERNOON

Section A

Hilton
Salon III

Refining and Petrochemicals Using Renewable Feedstocks
New Platform Chemicals and Chemical Building Blocks for Petrochemicals
Cosponsored by CATL (probationary)

B. H. Shanks, K. Fjare, and C. Zhang, *Organizers*

1:30 Introductory Remarks.
1:40 **4.** Changes in the energy market and their impact on the chemical industry. **B. R. Maughon**
2:30 **5.** Production of monofunctional hydrocarbons from biomass derived carbohydrates via catalytic conversion on carbon supported platinum-rhenium. **D. A. Simonetti**, E. L. Kunkes, R. M. West, J. C. Serrano-Ruiz, C. A. Gartner, J. A. Dumesic
2:55 Intermission.
3:10 **6.** Recent developments in the conversion of biomass to renewable fuels and chemicals. **L. Manzer**
4:00 **7.** Withdrawn.

Alternative Hydrocarbons: Tar Sands, Oil Shale, and Heavy Oil: Production, Processing, and Chemistry Sponsored by FUEL, Cosponsored by PETR‡

Nanotechnology in Catalysis VI Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, and NANO

MONDAY MORNING

Section A

Hilton
Salon III

Feedstock Allocation in Petroleum Refineries

C. S. Hsu and P. Robinson, *Organizers*

9:00 **8.** Allocation of nonconventional feedstocks in petroleum refineries: Overview. **P. Robinson**
9:25 **9.** Biofuels in China. **X. Hu**, H. Sun, X. Fu
10:10 Intermission.
10:25 **10.** Compositional analysis of heavy conventional crude oils: The definition of asphaltenes and maltenes by high resolution mass spectrometry. **R. P. Rodgers**, A. M. McKenna, A. G. Marshall
10:50 **11.** Separation and analysis of basic and nonbasic nitrogen compounds in vacuum gasoline. **H. Dulot**, N. Charon-Revellin, C. Lopez-Garcia, J. Jose
11:15 **12.** Characterization of basic nitrogen in heavy petroleum by microelectrospray 9.4T Fourier transform ion cyclotron resonance mass spectrometry. **Y. Liu**, Q. Hu, Z. Liu, X. Zhu, S. Tian

Nanotechnology in Catalysis VI Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, and NANO

MONDAY AFTERNOON

Section A

Hilton
Salon III

Feedstock Allocation in Petroleum Refineries

P. Robinson and C. S. Hsu, *Organizers*

2:00 Introductory Remarks.
2:10 **13.** VSEP membrane filtration for Canadian crudes. **M. Galimberti**
2:35 **14.** Molecular reconstruction of vacuum residues. **J. J. Verstraete**, H. Dulot, D. Hudebine
3:00 **15.** Gas chromatography for molecular mass determination of petroleum distillates. **L. Carbognani**, T. Oldenburg, L. Diaz Gomez, S. Larter, P. Pereira-Almao
3:25 Intermission.
3:40 **16.** Quantitative analysis and structural characterization of petroleum pitches. **S. U. Kulkarni**, M. C. Thies
4:05 **17.** Comparative compositional analysis of untreated and hydrotreated oil by GC field ionization time-of-flight high resolution mass spectrometry. **X. Zhu**, C. Li, Z. Liu, Y. Liu, S. Tian

Catalysis for Cellulosic Feedstock Conversion Sponsored by CATL (probationary), Cosponsored by CELL, COLL, FUEL, I&EC, and PETR

Nanotechnology in Catalysis VI Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, and NANO

MONDAY EVENING

Sci-Mix Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, and PETR

TUESDAY MORNING

Section A

Hilton
Salon III

Chemistry of Petroleum and Emerging Technologies
Sulfur Poisoning and Advances in Sulfur Removal Technologies

K. Fjare, *Organizer*

9:00 Introductory Remarks.
9:10 **18.** Synthesis and characterization of nanosized hydrodesulfurization (HDS) catalyst. **D. Mahajan**, M. Anjom, I. Dovgani
9:35 **19.** Impact of sulfur poisoning on the carbon deposition over Rh and Ni catalysts in steam reforming of liquid hydrocarbons. C. Xie, **Y. Chen**, Y. Li, X. Wang, C. Song

The official technical program for the 237th National Meeting is available online at oasys2.confex.com/acs/237nm/techprogram/.

10:00 20. Preparation and selective adsorption desulfurization activity of Ti-Ce-Al-Ag-O adsorbent. **F. Sun**, X. Ma, C. Song
10:25 Intermission.
10:35 21. Ultraclean fuels via modified ultrasound assisted oxidative desulfurization process. S. S. Cheng, **T. F. Yen**
11:00 22. Recent advances in biodesulphurization of fuels. **R. C. Nwokoma**

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Catalysis and Reaction Mechanisms
Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

Nanotechnology in Catalysis VI Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, and NANO

TUESDAY AFTERNOON

Section A

Hilton
Salon III

Chemistry of Petroleum and Emerging Technologies

K. Fjare, *Organizer*

2:00 Introductory Remarks.
2:10 23. Removal of carboxylic acids in Fischer-Tropsch hydrocarbon product. **F. H. A. Bolder**
2:35 24. The challenges for processing Canadian bitumen-derived crudes. **Z. Fan**, P. Rahimi, T. Alem
3:00 Intermission.
3:10 25. Total acid number determination in vacuum and atmospheric residue of petroleum using attenuated total reflectance Fourier transform infrared spectroscopy and different partial least squares algorithms. **E. I. Muller**, G. Parizotto, A. L. Hermes, M. F. P. dos Santos, R. C. L. Guimarães, M. F. Ferrão, É. M. M. Flores
3:35 26. Demulsification of heavy crude oils for salt extraction using closed vessels microwave heating and further chlorine determination by ion selective electrode or titration. É. M. Flores, **J. S. Pereira**, F. G. Antes, D. P. Moraes, L. O. Diehl, J. N. Paniz, V. L. Dressler, M. F. P. Santos, R. C. Guimarães

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Surface Chemistry of Oxides Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

Nanotechnology in Catalysis VI Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, and NANO

WEDNESDAY MORNING

Section A

Hilton
Grand Ballroom C

Poster Session

K. Fjare, *Organizer*

9:00–11:00
27. Total acid number distribution in a Brazilian refinery oil sample after exposure to different levels of heating in the process units. **A. D. O. Gomes**, R. C. L. Guimarães, I. P. Batista
28. Biosynthesis of the acid by a new technology and bioreactors. **F. Abniki**, E. Bakhshi
29. How comb-type poly(maleic acid alkylamide -co-alfa-olefin) assembles in waxy oils and improves cold flowing ability. X. Zhang, J. Xu, J. Sun, L. Li, **X. Guo**
30. Hydro processing rape seed oil with gas oil for diesel fuel. **B. Gevert**, J. Claesson, K. Holmgren, U. Kuylenstierna, B. Lundin, L. Nilsson, A. Sherif
31. Investigation of safe operation of exothermic reactions in chemical industries: Presenting procedure. **E. Bakhshi**, F. Abniki, M. Mosalla
32. Investigation of water quality with changing the method of microorganisms control. **E. Bakhshi**, F. Abniki
33. On the lumped parameter called efficiency in vapor distillation problems. **S. R. Kal**
34. Pilot test study of an ex-situ presulfided NiMo/Al2O3 catalyst. **Y. Li**, D. Liu
35. Solid base and their performance in synthesis of dipropylene glycol. **L. Lu**, Y. Xiang, D. Xia, Y. Zhou
36. Storing sensible heat by supporting phase change material, PCM. **F. Abniki**, E. Bakhshi
37. Synthesis of mesoporous ZSM-5 by inverse self-assembly of secondary unit. **L. Dai**, Z. Yan
38. Thermal cracking studies by design of a pilot plant. **F. Abniki**, E. Bakhshi, M. Mosalla, A. Bakhshi

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Bimetallics and Electrocatalysis Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

Nanotechnology in Catalysis VI Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, and NANO

WEDNESDAY AFTERNOON

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Cynthia M. Friend
Surface Characterization and Chemistry Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, WCC, and PHYS

Nanotechnology in Catalysis VI Sponsored by CATL (probationary), Cosponsored by COLL, FUEL, I&EC, PETR, and NANO

‡ **Cooperative Cosponsorship**

PHYS

Division of Physical Chemistry

M. Head-Gordon, *Program Chair*

SUNDAY MORNING

Section A

Salt Palace Convention Center
250 A

Advances in Electronic Structure Theory and First Principles Dynamics
Advances at the Interface of Electronic Structure and Dynamics

C. D. Sherrill and G. Galli, *Organizers, Presiding*

8:00 Introductory Remarks.
8:10 1. Photochemistry and mechanochemistry from first principles dynamics. **T. J. Martinez**
8:50 2. Predictive electronic structure methods for charge transfer systems. **A. I. Krylov**
9:30 3. Ab initio based potentials and dynamics using them. **J. M. Bowman**, B. J. Braams
10:10 Intermission.
10:30 4. Exploring electron transfer and bond breaking with constrained DFT. **T. Van Voorhis**
11:10 5. Developments in coupled-cluster molecular dynamics. **A. G. Taube**

Section B

Salt Palace Convention Center
250 B

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of Jens Norskov: Convergence between Theory and Experiment in Surface Chemistry and Catalysis

J. T. Yates Jr., *Organizer, Presiding*

8:00 Introductory Remarks.
8:10 6. Reactivity trends in cooxidation from uhv to elevated pressures. S. M. Mcclure, M. Lundwall, F. Yang, Z. Zhou, **D. W. Goodman**
8:50 7. Which transition states and intermediates control catalyst activity, and how well do we know their energies? **C. T. Campbell**
9:30 8. What can we learn from empirically determined kinetic parameters? **K. Reuter**
10:10 9. Award Address (Gabor A. Somorjai Award for Creative Research in Catalysis, sponsored by Gabor A. and Judith K. Somorjai Endowment Fund). Structural and electronic effects in the reactivity of metal surfaces. **J. K. Norskov**
10:50 10. Theoretical and experimental studies using model systems for the design of selective catalysts with well-defined shapes. I. Lee, F. Delbecq, **F. Zaera**
11:10 11. Olefins at oxide surfaces studied by vibrational sum frequency generation. **F. M. Geiger**, A. M. Buchbinder, G. Y. Stokes
11:30 12. Pathways and intermediates of formic acid decomposition on the CeO2(111) surface. **Y. Xu**, W. O. Gordon, S. D. Senanayake, D. R. Mullins, S. H. Overbury
11:50 13. DFT modeling of the interaction of noble metals with ceria and zirconia surfaces. **R. Grau-Crespo**, N. C. Hernandez, J. F. Sanz, N. H. de Leeuw

Section C

Salt Palace Convention Center
250 C

Functional Motions in Enzyme Catalysis
Cosponsored by BIOL

A. Kohen, *Organizer*

A. Warshel, *Organizer, Presiding*

8:30 Introductory Remarks.
8:35 14. A dynamic duo where rate constants, or selectivity are determined by tuning dynamic trajectories. **R. Stroud**, J. Finer-Moore, S. Hur, Z. Newby
9:15 15. What X-ray diffraction can—and can't—tell us about functional motions. **G. A. Petsko**
9:55 Intermission.
10:10 16. The missing atom in functional motion: Reliable determination of hydrogen positions. **D. Ringe**
10:50 17. Elucidating functional motions in a single protein crystal. **E. N. Brown**, S. Ramaswamy, B. V. Plapp
11:30 18. Insight into RNA catalysis by hammerhead ribozyme from QM/MM free-energy profile simulations. **K-Y. Wong**, T-S. Lee, D. M. York

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

Section D

Salt Palace Convention Center
Combo Rooms 250 D&E

Molecular Hydrogen in Nanoporous Materials: Meeting Ground for Theory and Experiment
Accurate Calculation of Interactions of Dihydrogen with Nanoporous Materials
Cosponsored by NANO

M. D. Ward, *Organizer*

Z. Bacic, *Organizer, Presiding*

8:00 Introductory Remarks.
8:10 19. Accurate quantum chemical calculation of the interaction of dihydrogen with hydrogen-storage materials. **W. Klopper**, A. Mavrandonakis
8:50 20. Electronic structure methods for hydrogen storage calculations. **M. Head-Gordon**
9:30 21. Simulation of free energies of hydrogen adsorption in nanoporous systems with quantized molecular-fluid DFT. **S. Patchkovskii**, T. Heine
10:10 Intermission.
10:30 22. H2 generation and storage on nanoporous materials: Theoretical studies and new development. **S. Meng**
11:10 23. The physics of hydrogen clusters: Structure, superfluidity and quantum melting. **M. Boninsegni**

Section E

Salt Palace Convention Center
251 B

Chemical Methods of Nanofabrication
Cosponsored by NANO‡

Y. H. Wang and S-J. Park, *Organizers*

C. A. Mirkin, *Presiding*

8:30 24. Crystals as molecules. **O. M. Yaghi**
9:05 25. New nanofabrication strategies: Inspired by biomineralization. **J. Aizenberg**, B. Pokroy, S. H. Kang, A. Epstein
9:40 26. Cooperative self-assembly of nanoparticles and amphiphilic block-copolymers in selective solvents. **S-J. Park**, B. L. Sánchez-Gaytán, R. Hicky, A. Kamps
10:15 Intermission.
10:25 27. Controlling the synthesis and assembly of nanoscale building blocks. **Y. Xia**
11:00 28. Directing nanoparticle nucleation and assembly using self-assembled peptide conjugates. **N. L. Rosi**, C. Chen, P. Zhang

Section F

Salt Palace Convention Center
251 C

Progress in Polarizable Force Fields and Simulation
Large Scale Polarizable Force Field Development

T. Head-Gordon, *Organizer*

V. S. Pande, *Organizer, Presiding*

8:00 29. Fluctuating charge force fields for protein simulations. **C. L. Brooks III**
8:40 30. Calibration and validation of the AMOEBA polarizable force field. **J. W. Ponder**
9:20 31. Classical force field development: What can we learn from carbohydrates? **R. J. Woods**
10:00 Intermission.
10:20 32. Optimization of a polarizable force field based on the classical Drude oscillator and application to biological macromolecules. **A. D. MacKerell Jr.**
11:00 33. Polarizable modeling of proteins: Force fields and empirical corrections. **R. A. Friesner**