

**Energy & Fuels Preprints  
Presented at the 248th  
ACS National Meeting &  
Exhibition 2014**

**Division of Energy & Fuels, American Chemical Society  
Energy & Fuels Preprints Volume 59 #2**

**San Francisco, California, USA  
10-14 August 2014**

**ISBN: 978-1-63266-923-0**

**Printed from e-media with permission by:**

Curran Associates, Inc.  
57 Morehouse Lane  
Red Hook, NY 12571



**Some format issues inherent in the e-media version may also appear in this print version.**

Copyright© (2014) by American Chemical Society Division of Energy and Fuels  
All rights reserved.

Printed by Curran Associates, Inc. (2014)

For permission requests, please contact American Chemical Society Division of Energy and Fuels  
at the address below.

American Chemical Society Division of Energy and Fuels  
c/o Dr. Elise B. Fox  
Savannah River National Lab  
Materials Science and Technology  
Aiken SC 29809

Phone: (803) 507-8560

Elise.fox@srnl.doe.gov

**Additional copies of this publication are available from:**

Curran Associates, Inc.  
57 Morehouse Lane  
Red Hook, NY 12571 USA  
Phone: 845-758-0400  
Fax: 845-758-2634  
Email: curran@proceedings.com  
Web: www.proceedings.com

# Table of Contents

Please Click on Symposia to View Related Papers

## 1. Hydrogen Generation and Hydrogen Based Global Economy

<b>Role of interface between metal and support on steam reforming of toluene over Ni/LSAO-perovskite catalyst</b>	<b>1</b>
Daiki Mukai, Kento Takise, Masaya Imori, Shuhei Ogo, Yukihiro Sugiura, Yasushi Sekine	
<b>Theoretical and Experimental Understanding on Ethanol Steam Reforming for H<sub>2</sub> Production</b>	<b>3</b>
Jia Zhang, Ziyi Zhong, X.-M. Cao, P. Hu, Michael Sullivan, Luwei Chen	
<b>Material investigation for hydrogen production and storage applications: Hydrogen solubility in transition metals predicted by density functional theory combined with thermodynamic principles</b>	<b>5</b>
Kyoungjin Lee, Mengyao Yuan, Antonio Baclig, Jennifer Wilcox	
<b>Catalytic methane steam reforming in an electric field at low temperature</b>	<b>8</b>
Ryo Manabe, Kazumasa Oshima, Yusuke Sasaki, Shuhei Ogo, Yasushi Sekine	
<b>B-N compounds for hydrogen storage: What's left to learn?</b>	<b>10</b>
R. Tom Baker	
<b>Manipulating photogenerated electrons and holes in semiconductors for solar hydrogen production</b>	<b>12</b>
Peng Zhang, Jinlong Gong	
<b>High-pressure storage of hydrogen fuel: Ammonia borane and its related compounds</b>	<b>14</b>
Yu Lin, Wendy Mao	
<b>RATIONALLY DESIGNED CuFe<sub>2</sub>O<sub>4</sub> – MESOPOROUS Al<sub>2</sub>O<sub>3</sub> COMPOSITE TOWARDS STABLE PERFORMANCE OF HIGH TEMPERATURE WATER-GAS SHIFT REACTION</b>	<b>15</b>
Chinnakonda Gopinath, Hyun-Seog Roh	
<b>Steam reforming of ethanol over Co/K/<math>\alpha</math>-Al<sub>2</sub>O<sub>3</sub> catalyst</b>	<b>17</b>
Shuhei Ogo, Takuya Shimizu, Yusaku Nakazawa, Kei Mukawa, Daiki Mukai, Yasushi Sekine	
<b>Ethanol Steam Reforming over Cobalt Catalysts Supported on Nano-ceria: Oxidation/reduction Behavior of the Metal and the support</b>	<b>19</b>
Umit Ozkan, I. Ilgaz Soykal, Hyuntae Sohn, Jeffrey Miller	
<b>Oxidation resistance and effect of Pt addition to Ni/La<sub>0.7</sub>Sr<sub>0.3</sub>AlO<sub>3-<math>\delta</math></sub> for catalytic steam reforming of toluene for hydrogen production</b>	<b>20</b>
Yukihiro Sugiura, Daiki Mukai, Masaya Imori, Takashi Hashimoto, Shuhei Ogo, Yasushi Sekine	
<b>Study about the effect of gadolinium doped ceria as support material for copper oxide to remove carbon monoxide in hydrogen rich stream</b>	<b>23</b>

Jiwoo Oh, Joongmyeon Bae

<b>Novel approaches to carbon nitride photocatalysts for enhanced H<sub>2</sub> evolution</b>	<b>25</b>
Dariya Dontsova, Christian Fettkenhauer, Markus Antonietti, Guylhaine Clavel	
<b>Catalytic activation of liquid-phase chemical hydrides for hydrogen generation</b>	<b>26</b>
Qiang Xu	
<b>Sorbent enhanced methane reforming over a Ni-Ca-based, bi-functional catalyst sorbent</b>	<b>27</b>
Marcin Broda, Agnieszka Kierzkowska, David Baudouin, Qasim Imtiaz, Christophe Copéret, Christoph Müller	
<b>Polymer Dye-Sensitizer for Photoelectrochemical Water Splitting</b>	<b>29</b>
Raman Vedarajan, Shoto Ikeda, Noriyoshi Matsumi	
<b>Pyrolysis of biomass in a bench-scale downer reactor combined with secondary decomposition for production of hydrogen-rich gas</b>	<b>30</b>
Tongli Ding, Yongwei Wang, Songgeng Li, Wenli Song, Weigang Lin	
<b>Hydrogen production from landfill gas</b>	<b>32</b>
Sania de Lima, Raimundo Rabelo-Neto, Claudio Mahler, Adriana de Schueler, Fabio Noronha	
<b>X-ray spectroscopy (XAS) studies of Fe-Cu based oxygen carriers for a chemical looping based hydrogen production cycle</b>	<b>33</b>
Qasim Imtiaz, Nur Sena Yüzbası, Agnieszka Kierzkowska, Paula Abdala, Wouter van Beek, Christoph Müller	
<b>Desulfurization of H<sub>2</sub>S using porous ZnO-based materials as sorbents</b>	<b>35</b>
Dat Tran, Charles Rong	
<b>Hydrogen and Liquid Fuel Co-Generation via a Cyclic Redox Scheme</b>	<b>37</b>
Fanxing Li, Feng He	
<b>Use of catalysts to promote the activity of weak metal hydroxides in the alkaline thermal treatment of cellulose to H<sub>2</sub></b>	<b>38</b>
Ah-Hyung Park, Maxim Stonor	

## **2. Biofuels for Powering the World**

<b>Hydrogenation of lactic acid to propylene glycol over Mo modified Ru/C catalyst</b>	<b>40</b>
Yasuyuki Takeda, Tomohiro Shoji, Masazumi Tamura, Yoshinao Nakagawa, Keiichi Tomishige	
<b>Catalytic conversion of lignin to hydrocarbon fuels</b>	<b>42</b>
Xiaodong Tian, Yueyuan Ye, Yunquan Liu	
<b>Hydrogeonolysis of squalane over novel metal catalysts</b>	<b>44</b>
Shin-ichi Oya, Daisuke Kanno, Hideo Watanabe, Masazumi Tamura, Yoshinao Nakagawa, Keiichi Tomishige	
<b>Improved catalyst for fatty acid deoxygenation to hydrocarbon biofuels</b>	<b>46</b>
Keyi Sun, Adria Wilson, Simon Thompson, H. Lamb	

<b>Kinetics of <math>\gamma</math>-valerolactone formation during aqueous phase hydrogenation of levulinic acid over supported Ru</b>	<b>48</b>
Jesse Bond, Omar Abdelrahman	
<b>The Hydrodeoxygenation of Bioderived Furans into Alkanes: Process Development</b>	<b>49</b>
Amanda King, John Gordon, Andrew Sutton	
<b>Simultaneous Conversion of Biomass and CO<sub>2</sub> to Co-produce Carboxylic Acids by Aqueous-phase Hydrogen Transfer</b>	<b>51</b>
Hongfei Lin	
<b>Performance of Solid Acid-Base Catalysts for Production of Acrolein by Gas-Phase Dehydration of Aqueous Glycerol</b>	<b>53</b>
Bo-Qing Xu	
<b>Hydrotreating of biomass pyrolysis oils in the presence of solvents</b>	<b>54</b>
Richard French, Luc Moens, James Stunkel, Kristiina Iisa	
<b>HYDROGENOLYSIS OF C-O BONDS IN BIOMASS-BASED SUBSTRATES USING Ir-ReO<sub>x</sub>/SiO<sub>2</sub> CATALYSTS: ROLE OF Re SPECIES AND ACID COCATALYSTS</b>	<b>58</b>
Keiichi Tomishige	
<b>Oxidative Depolymerization and Stabilization of Lignin-Derived Bio-oils</b>	<b>60</b>
R. Tom Baker, Cedric Briens, Baburam Sedai, Jin Lin Zhou	
<b>Hydrodeoxygenation of fast pyrolysis oil using Ru/C catalyst-effects of solvents</b>	<b>62</b>
Shima Ahmadi, Ehsan Reyhanitash, Cheng Guo, Zhongshun Yuan, Guus Van Rossum, Sohrab Rohani, Chunbao (Chalres) Xu	
<b>Bio-Crude Upgrading Over Early Transition Metal Carbide And Nitride-Based Catalysts</b>	<b>64</b>
Levi Thompson, Allison Franck, Sarah Paleg	
<b>Lignin into arenes: A new platform for the production of liquid fuels by catalytic H-transfer reactions</b>	<b>65</b>
Roberto Rinaldi, Xingyu Wang	
<b>Aging process of biomass pyrolysis oil and its model compounds – a mechanistic study</b>	<b>67</b>
Haoxi Ben, Mark Jarvis, Mark Nimlos, David Robichaud, Calvin Mukarakate, Steve Deutch	
<b>Catalytic Requirements for the Deoxygenation of Aldehydes and Ketones on Solid Brønsted Acid Catalysts</b>	<b>69</b>
Ya-Huei (Cathy) Chin, Fan Lin	
<b>Role of pericyclic reactions in the pyrolysis of cellulose and hemicellulose</b>	<b>71</b>
Phillip Westmoreland, Vikram Seshadri, Patrick Fahey	
<b>Role of Bifunctional Catalysts in the Hydropyrolysis of Lignin</b>	<b>73</b>
Fernando Resende, Eranda Nikolla, Oliver Jan, Layan Savithra, Ryan Marchard, Luiz Carlos Araújo dos Anjos	
<b>Intermediate radicals from thermal degradation of p-coumaryl alcohol in the gas</b>	<b>75</b>

**phase**

Lavrent Khachatryan, Rubik Asatryan, Alexander Baev, Barry Dellinger

**Effect of Pore-Structure on Production of Furans and Value Added Chemicals From Biomass 76**

SRIDHAR BUDHI, CALVIN MUKARAKATE, MARK NIMLOS, BRIAN TREWYN

**Catalyst deactivation in ex situ and in situ catalytic fast pyrolysis of biomass 78**

Kristiina Iisa, Alexander Stanton, Mark Nimlos

**Upgrading biomass pyrolysis products using five different catalysts; effect on product speciation and coking rates 80**

Calvin Mukarakate, Sridhar Budhi, Kristiina Iisa, Mark Nimlos, David Robichaud

**Upgrading biomass-derived pyrolysis vapors on catalysts of varying acidity 81**

Matthew Yung, Calvin Mukarakate, Chaiwait Engtrakul, Anne Starace

**Selective Hydrogenation of biomass Pyrolysis vapors 82**

Mark Nimlos, Calvin Mukarakate, David Robichaud, Rhodri Jenkins

**Assessing the Suitability of Different Biomass Feedstocks for Processing via Gasification 84**

Matthew Boot-Handford, Nick Florin, Rafael Kandiyoti, Paul Fennell

**Electrofermentation to Produce Fuels from Carbon Dioxide 90**

Daniel Derr, Rahul Mirani, Gregg Deluga, Nattaporn Lohitharn

**Technical assessment for the production of cellulosic ethanol from sugarcane bagasse at high total solids and low enzyme loadings 92**

Luiz Ramos, Marcos Silveira, Priscila Neves, Luana Chiarello, Mateus Urio, Larissa da Silva

**Homogeneous catalysts stabilized in ionic liquids for processing biomass and biomass-derived chemicals 94**

Girish Srinivas, Michael Mundschau, Jeffrey Martin, Steven Gebhard

**Engineering of bacterial methyl ketone synthesis for biofuels: Recent advances 97**

Harry Beller, Ee-Been Goh, Edward Baidoo, Jay Keasling

**Hydrocarbons produced from a sterol rich microbial lipid isolated from an oleaginous yeast cultured in non-sterile conditions 98**

Christopher Chuck, Fabio Santomauro, Jonathan Wagner, Rod Scott

**Low Cost Ionic Liquids for Biorefining 102**

Jason Hallett, Agnieszka Brandt

**Sequential phototrophic to heterotrophic algal cultivation strategy for high-productivity lipid production 104**

Hamid Rismani-Yazdi, Kristin Hampel, Chris Lane, F. C. Thomas Allnut

**Molecular-level interactions in the design of reversible and recyclable flocculants 106**

Kathryn Morrissey, Chunlin He, Rebecca Chapman, Lucjan Żołnierowski, Mark Stoykovich

**Design of liquid reaction media and extractant for efficient 107**

<b>5-hydroxymethylfurfural production from glucose</b>	
Z. Conrad Zhang, Tingyu Huang, Jinxia Zhou, Songyan Jia, Zhi Xia, Kairui Liu, Wenjuan Xu, Peifang Yan	
<b>Conversion of cellulosic biomass catalyzed by activated carbons</b>	<b>108</b>
Atsushi Fukuoka	
<b>Catalytic Transformations of Cellulose and Cellulose-derived Carbohydrates into Organic Acid</b>	<b>110</b>
Ye Wang, Yanliang Wang, Zhenchen Tang, Weiping Deng, Qinghong Zhang	
<b>Biomass Derived Small Oxygenates to Fuel Range Hydrocarbons over HZSM-5</b>	<b>112</b>
Yong Wang, Karthikeyan Ramasamy	
<b>Ultra-Selective Cycloaddition of Dimethylfuran for Renewable p-Xylene with H-BEA Zeolite</b>	<b>114</b>
Wei Fan, Chun-Chih Chang, Paul Dauenhauer	
<b>On the promoting effects of salts upon acid-catalyzed hydrolysis of 1,4-<math>\beta</math>-glucans</b>	<b>116</b>
Heitor Fernando de Oliveira, Roberto Rinaldi	
<b>Upgrading Carbohydrates into Hydrocarbons For Fuels Applications</b>	<b>118</b>
John Gordon, Amanda King, Pete Silks, Andrew Sutton, Ruilian Wu	
<b>Direct catalytic conversion of cellulose to a liquid mixture of paraffins and naphthenes</b>	<b>120</b>
Beau Op de beeck, Michiel Dusselier, Jeroen Snelders, Christophe Courtin, Steffen Oswald, Lars Giebelier, Pierre Jacobs, Bert Sels	
<b>Kinetic study on glucose transformation to ethylene glycol_Part I: retro-aldol condensation</b>	<b>121</b>
Junying Zhang, Baolin Hou, Hua Wang, Aiqin Wang, Mingyuan Zheng, Jifeng Pang, Tao Zhang	
<b>Performance of a Diesel Power Generator Fuelled by Diesel Oil-Ethanol Blends</b>	<b>123</b>
Alex de Oliveira, André Morais, João Januário, Osmano Valente, José Sodré	
<b>Raw biogas purification by supported liquid membranes</b>	<b>127</b>
Pavel Izák, Zuzana Sedláková, Lenka Morávková, Karel Friess	
<b>Compressed-liquid densities of two alternative turbine fuels</b>	<b>129</b>
Stephanie Outcalt, Raina Gough, Thomas Bruno	
<b>Unimolecular decomposition of common radical intermediates found in oxygenated fuels</b>	<b>131</b>
Enoch Dames, Shamel Merchant, William Green	
<b>Reduction of Carbon Dioxide Emissions from Automobile Engine Using Ethanol as Fuel</b>	<b>133</b>
Leandro Almeida, Luis Carlos Sales, José Sodré	
<b>Comparative life cycle assessment of two C4 energy crops for power generation</b>	<b>138</b>
Xinhua Shen, Samarita Sarker, Ziaul Huque, Raghava Kommalapati	

**Impact of Fuel and Injection Timing on Partially-Premixed Charge Compression Ignition (PCCI) Combustion Mode** **139**

Andre Boehman, Chenxi Sun, Dongil Kang, Stani Bohac

### **3. Carbon-Based Materials for Energy Conversion and Storage**

**Semiconducting Carbon Nanotube Aerogel Bulk Heterojunction Solar Cells** **142**

Yumin Ye, Dominick Bindl, Robert Jacobberger, Meng-Yin Wu, Michael Arnold, Susmit Singha Roy

**Mechanochemically driven edge-selectively functionalized graphene nanoplatelets and their uses as electrocatalysts for energy conversion** **143**

In-Yup Jeon, Jeong-Min Seo, Jong-Beom Baek

**Investigation of silica supported fullerene catalysts for oxidative dehydrogenation of alkanes** **145**

Ibrahim Ilgaz Soykal, Viviane Schwartz, Hui Wang, Chengdu Liang

**Nitrogen and boron co-doped graphene as efficient catalyst for oxygen reduction reaction** **147**

Yiyi She, Michael Leung

**On the options for Hydrogen storage** **148**

Balasubramanian Viswanathan

**BIOMASS-DERIVED POROUS CARBONACEOUS MATERIALS FOR BIOFUELS PRODUCTION** **150**

Rick Arancon, Antonio Romero, Rafael Luque

**In situ One-Step Synthesis of Hierarchical Nitrogen-Doped Porous Carbon for High Performance Supercapacitors** **151**

Ju-Won Jeon, Satish Nune, Jodie Lutkenhaus

**Interconnected Carbon Nanosheets Derived from Hemp for Ultrafast Supercapacitors with High Energy** **152**

David Mitlin

**Graphene and Related Materials for Energy Storage** **155**

Rodney Ruoff

**Solid-State Supercapacitor Based on Activated Carbon Cloths Exhibits Excellent Rate Capability** **156**

Yat Li

**Roll-to-Roll Synthesis of Vertically Aligned Carbon Nanotube Electrodes for Electrical Double Layer Capacitors** **157**

Margarita Arcila-Velez, Jingyi Zhu, Anthony Childress, Mehmet Karakaya, Ramakrishna Podila, Apparao Rao, Mark Roberts

**Highly active iron and nitrogen doped carbon catalyst with hollow core mesoporous shell structure toward oxygen reduction reaction (ORR)** **159**

Ming Zhou, Kwong Chan

**Properties needed of carbon based anodes for use Sodium Ion Batteries.** **161**



Clement Bommier, Wei Luo, Xiulei Ji, Jenna Schardt, John Simonsen

<b>Carbon in Primary Lithium Air Batteries</b>	<b>163</b>
Jie Xiao	
<b>Carbonaceous materials as CO<sub>2</sub> adsorbent: Design and simulation</b>	<b>164</b>
De-en Jiang	
<b>Colossal pseudocapacitance in a high functionality - high surface area carbon anode doubles the energy of an asymmetric supercapacitor</b>	<b>165</b>
David Mitlin	
<b>Advanced lithium-sulfur batteries from graphene-based architectures</b>	<b>167</b>
Quan-Hong Yang	
<b>Salt templating: Carbons with precise nanoporosity and their application as advanced supercapacitors</b>	<b>168</b>
Nina Fechler, Girum Tiruye, Rebeca Marcilla	
<b>Bi-functional electrocatalyst based on Cu-Fe alloy and highly crystalline carbon sheets for rechargeable Zn-air battery.</b>	<b>169</b>
Gyutae Nam, Jaephil Cho	
<b>Carbon composite non-precious metal catalysts for oxygen reduction in electrochemical energy conversion</b>	<b>170</b>
Piotr Zelenay, Hoon Chung, Edward Holby, Christopher Taylor, Gang Wu	
<b>Building energy- and size-scalable three-dimensional energy-storage architectures with carbon nanofoam paper</b>	<b>172</b>
Debra Rolison, Megan Sassin, Jeffrey Long, Jean Wallace, Christopher Chervin	
<b>Graphene Materials for High-Performance Supercapacitors: Two Dimensional or Three Dimensional?</b>	<b>175</b>
Yanwu Zhu	
<b>Nitrogen-doped carbon networks derived from polyaniline coated bacterial cellulose for high energy density supercapacitors</b>	<b>176</b>
Jun Yan, Tong Wei, Zhuangjun Fan	
<b>Functionalized carbon nanostructures for electric energy storage</b>	<b>178</b>
Y.Y. Shao, J. Liu, Y.H. Lin	
<b>Fabrication and Characterization of Platinum Coated with Solution Processed Graphene</b>	<b>179</b>
Yinghe Zhang	
<b>Synthesis of structured carbon particles in an electric field and its application</b>	<b>181</b>
Kei Mukawa, Naganobu Oyama, Hiroaki Ando, Takashi Sugiyama, Shuhei Ogo, Yasushi Sekine	
<b>Durable Pd@Pt core-shell Electrocatalyst for proton exchange membrane fuel cells (PEMFCs)</b>	<b>183</b>
zhigang Shao	

<b>Porous carbon nanosheets with precisely tunable thickness for use in high rate and long cycle life supercapacitors</b>	<b>184</b>
Wen-Cui Li, Zhen-Yu Jin, Xiang-Qian Zhang	
<b>High Efficient Reversible Hydrogen Storage-Evolution Process Based on Redox Ammonium Bicarbonate (or Carbamate)/Formate Equilibrium over Pd NPs Catalyst</b>	<b>186</b>
Ji Su, Lisha Yang, Xiaokun Yang, Mi Lu, Hongfei Lin	
<b>Rational Nanostructured Carbon for Energy Conversion and Storage</b>	<b>187</b>
Liangbing Hu	
<b>Design Principles to Exceed the DOE 2017 Standards for Delivery and Storage of H<sub>2</sub> at Room Temperature Using nitrogen bases Covalent Organic Frameworks.</b>	<b>188</b>
Jose Mendoza-Cortes, William Goddard III, Hiroyasu Furukawa, Omar Yaghi	
<b>Scalable Synthesis of 3D Heteroatom-doped Carbon Nanofibers from Bacterial Cellulose for Supercapacitors</b>	<b>189</b>
Li-Feng Chen, Shu-Hong Yu	

#### **4. Metal-Organic Frameworks for Sustainable Energy**

<b>High volumetric uptake in aluminum metal-organic frameworks</b>	<b>191</b>
Omar Yaghi	
<b>MOF-based catalysts for lignin degradation</b>	<b>193</b>
Mark Allendorf, Ryan Davis, Parthasarathi Ramakrishnan, Kenneth Sale, Vitalie Stavila	
<b>Metal-Organic Frameworks from Design Strategies to Applications</b>	<b>194</b>
Mohamed Eddaoudi	
<b>Generating Highly Reactive and Highly Stable Catalysts by Combining Molecular and Material Chemistry</b>	<b>195</b>
Sid Das, Rebecca Hansen, Marina Popova, Moumita Bhattacharya	
<b>Demystifying Paths to MOF Commercialization</b>	<b>196</b>
Benjamin Hernandez	
<b>MOFs for use in mixed matrix membranes, produced at scale</b>	<b>197</b>
Matthew Hill, Cher Hon Lau, Marta Rubio-Martinez, Ravichandar Babarao, Stefan Smith, Bradley Ladewig, Anita Hill, Michael Batten, Kok-Seng Lim	
<b>Novel porous coordination polymers from a self-polymerizing phosphonium zwitterion and <i>bis</i>(phosphine) MCl<sub>2</sub> complexes</b>	<b>199</b>
Alisha Bohnsack, Nolan Waggoner, Graham Piburn, Bradley Holliday, Simon Humphrey	
<b>MOFs: Nanosized windows into Ångstrom space</b>	<b>201</b>
Christian Doonan, Christopher Sumbly, Witold Bloch	
<b>Adsorption-Based Heat Pumps: Energy Efficient Air-Conditioning with Microporous Metal-Organic Frameworks</b>	<b>203</b>
Mircea Dinca, Casey Wade, Minyuan Li, Tachmajal Corrales-Sanchez	
<b>High proton conductivity of novel zinc oxalate metal-organic frameworks having</b>	<b>204</b>

<b>pyridinium</b>	
Teppey Yamada, Takuya Nankawa	
<b>Metal-organic frameworks: towards the application to clean energy</b>	<b>205</b>
Qiang Xu	
<b>Metal-Organic Frameworks and their Nanocomposites for Carbon Fixation and Photo Catalysis</b>	<b>206</b>
Bo Wang, Yifa Chen, Rui Li, Changwen Hu	
<b>Extended metal-carbohydrate frameworks</b>	<b>207</b>
Fraser Stoddart	
<b>Directional energy transfer and charge transport within light-harvesting metal-organic framework materials</b>	<b>208</b>
Joseph Hupp	
<b>FUNCTIONAL METAL-ORGANIC FRAMEWORKS: "THE OTHER FMOFs"/FMOFs 2.0</b>	<b>209</b>
Mohammad A. Omary	
<b>Pore Engineering of Metal-Organic Frameworks for Hydrogen Storage and Carbon Capture</b>	<b>210</b>
Myunghyun Paik Suh	
<b>Porous Organic Materials for Electric Energy Storage and Power Supply</b>	<b>211</b>
Donglin Jiang, Fei Xu	
<b>Processing of metal-organic frameworks for air filtration applications</b>	<b>213</b>
Jared DeCoste, Gregory Peterson	
<b>Highly selective adsorption and separation of energy-related gases on soft metal-organic frameworks</b>	<b>214</b>
Ryotaro Matsuda, Hiroshi Sato, Susumu Kitagawa	
<b>Direct Synthesis of Isostructural Zirconium-Based Metal-Organic Frameworks as Methane Sorbents</b>	<b>215</b>
Hong-Cai Zhou, Xuan Wang	
<b>Molecular modeling of metal-organic frameworks for CO<sub>2</sub> capture</b>	<b>216</b>
Randall Snurr	
<b>Metal-organic frameworks as cathode materials for Li-O<sub>2</sub> battery</b>	<b>217</b>
Qiaowei Li, Doufeng Wu, Yong-gang Wang	
<b>How accurate are MOF crystal structures? Insight from DFT calculations</b>	<b>218</b>
David Sholl, Dalar Nazarian, Jeff Camp	
<b>Metal-organic frameworks for on-board storage of hydrogen and natural gas</b>	<b>219</b>
Eric Bloch, Jarad Mason, Matthew Kapelewski, Kenji Sumida, Miguel Gonzalez, Mercedes Taylor, David Gygi, Wendy Queen, Jinxing Ye, Jeffrey Long	
<b>Thermodynamic Assessment of the Ethylene - Bond Interactions with Open Metal Sites of MOF Materials.</b>	<b>220</b>

<b>Efficient light gas separations with MOFs <i>via</i> predictive modeling and tuned synthesis</b>	<b>221</b>
---	------------

Tina Nenoff

## **5. 3rd International Symposium on Graphene for Energy and Fuel**

<b>Insights into molecular transport through graphene and graphene-oxide membranes from simulation</b>	<b>222</b>
--	------------

De-en Jiang

<b>Hybrid Device Employing 3D Arrays of MnO in Carbon Nanosheets Bridges Battery - Supercapacitor Divide</b>	<b>223</b>
--	------------

David Mitlin

<b>Thermal and surface properties of graphene laminates for solar energy applications</b>	<b>226</b>
---	------------

Giovanni Fanchini, Sabastine Ezugwu, M. Shafiq Ahmed, Arash Akbari-Sharbafe, Reg Bauld, Faranak Sharifi

<b>Self-Assembled 3D Graphene Oxide Electrodes for Lithium-Ion Batteries</b>	<b>227</b>
--	------------

Tianyuan Liu, Reza Kaviani, Seung Woo Lee

<b>Illuminating Graphene</b>	<b>229</b>
------------------------------	------------

Andrea Ferrari

<b>Integration of carbon nanomaterials into heterostructure devices</b>	<b>230</b>
---	------------

Mark Hersam

<b>Graphene in Li-O<sub>2</sub> and Li-CF<sub>x</sub> Batteries</b>	<b>231</b>
---	------------

Jie Xiao

<b>Synthesis of porous carbon nanofibers for high-performance rechargeable lithium-sulfur batteries</b>	<b>232</b>
---	------------

An-Hui Lu, Xiang-Qian Zhang, Qiang Sun, Wen-Cui Li, Bin He

<b>Shape-control of 3D Graphene for Energy Application</b>	<b>234</b>
--	------------

Liang Chang, Wei Wei, Yun Hang Hu

<b>Graphene based materials for capacitive energy storage</b>	<b>235</b>
---	------------

Majid Beidaghi, Yury Gogotsi

<b>3D characterization of graphene oxide membranes using electron tomography</b>	<b>236</b>
--	------------

Ilke Arslan, Toby Sanders, Yongsoo Shin, Leonard Fifield, Birgit Schwenzer, Dongsheng Li, Wei Liu, Ram Devanathan, David Gotthold

<b>Graphene Supercapacitors: Charging Up the Future</b>	<b>237</b>
---	------------

Maher El-Kady, Jee Youn Hwang, Lisa Wang, Mengping Lee, Yuanlong Shao, Mir Mousavi, Jang Myoun Ko, Richard Kaner

<b>Chemical Functionalization of Graphene for Electrochemical Energy Storage</b>	<b>238</b>
--	------------

Ting Yu

<b>Co-doped graphene metal-free electrocatalysts for key energy conversion processes</b>	<b>241</b>
Shi Zhang Qiao, Yao Zheng, Yan Jiao	
<b>Mesoporous copper-doped cobalt oxide for high-performance supercapacitors</b>	<b>243</b>
Mir F. Mousavi, Richard B. Kaner, Afshin Pendashteh, Mohammad S. Rahmanifar	
<b>Graphene-Nickel Cobaltite Nanocomposite Asymmetrical Supercapacitor with Commercial Level Mass Loading</b>	<b>244</b>
David Mitlin	
<b>Graphene wrapping for lithium-sulfur batteries</b>	<b>246</b>
Chongwu Zhou, Jiepeng Rong, Mingyuan Ge, Xin Fang	
<b>Chemically Integrated Graphene/Inorganic Hybrid 2-D Materials for Flexible Energy Storage Devices</b>	<b>247</b>
Guihua Yu	
<b>Graphene and graphene-based materials: Synthesis and electrochemical energy applications</b>	<b>248</b>
Yuyan Shao	
<b>Interface induced 2D or 3D graphene assembly for energy storage</b>	<b>249</b>
Quan-Hong Yang	
<b>Sodium niobate nanotubes – Graphene and Sodium niobate nanorods – Graphene binder free nanocomposite flexible paper electrode for supercapacitors</b>	<b>250</b>
Wijayantha Perera, Kenneth Balkus	
<b>High-throughput production of graphene using supercritical fluid for energy applications</b>	<b>253</b>
Takaaki Tomai, Nobuto Oka, Naoki Tamura, Itaru Honma	
<b>How stable is graphene oxide for Photocatalytic Applications? Reactivity towards hydroxyl radicals</b>	<b>254</b>
James Radich, Prashant Kamat	
<b>6. 1st United States-China Symposium on Energy</b>	
<b>Graphene-metal oxide hybrid materials with high capacitance</b>	<b>255</b>
Zonghuai Liu, Liping Kang, Zhibing Lei	
<b>Rechargeable lithium sulfur batteries with novel sulfur-based cathode materials</b>	<b>257</b>
Jinbao Zhao, Bo Liu, Xuxiang Wang, Xue Li, Jing Wang, Chunmei Shi	
<b>Achieving low overpotentials in metal-air batteries</b>	<b>258</b>
Yiyi Wu	
<b>Porous carbon-modified hybrid anodes for lithium ion batteries</b>	<b>259</b>
Fei Han, Wen-Cui Li, Cheng Lei, Bin He, Qiang Sun, An-Hui Lu	
<b>Energy storage materials of Vanadate System</b>	<b>261</b>
Kongjun Zhu	

<b>Graphene-based electrode material design and preparation process for rechargeable battery application</b>	<b>262</b>
Zi-Feng Ma, Dezhi Yang, Tao Yuan, Yu-Shi He, Xiao-Zhen Liao	
<b>Coal to Liquid Conversion via Dimethyl Ether</b>	<b>263</b>
Chang-jun Liu, Xintong Zhou	
<b>Low-carbon energy solution in China</b>	<b>264</b>
Yuhan SUN, Zhiyong Tang	
<b>Mesopore structure controlled conversion and products selectivity in the design of heavy oil catalytic cracking catalyst</b>	<b>265</b>
Baojian Shen, Shuo Mi, Dongdong Guo, Zhenxing Qin, Shenyong Ren, Qiaoxia Guo, Hongjuan Zhao, Baojie Wang, Honghai Liu, Xionghou Gao	
<b>Hierarchical porestructure enhanced hydrocarbon catalytic cracking activity of ZSM-5 catalyst</b>	<b>267</b>
Xiaohui Li, Deheng Yang, Shenyong Ren, Qiaoxia Guo, Baojian Shen	
<b>Bringing New Efficiencies in Petroleum Refining Processes: In Silico Investigation on the Potential of Novel Porous Materials for Olefin and Paraffin Separation</b>	<b>269</b>
Loredana Valenzano, Gemechis Degaga, Kapil Adhikari	
<b>Synthesis of ethanol via hydrogenation of acetic ester on Cu/SiO<sub>2</sub>: Enhanced activity and stability with plasma treatment</b>	<b>270</b>
Yuan Liu, Jihong Cheng, Shetian Liu, Wei Di, Shuxun Tian, Qi Sun	
<b>Bifunctional Catalysts for Hydrogen and Oxygen Chemistry</b>	<b>271</b>
Douglas Grotjahn	
<b>Investigating Photo-driven Heterogeneous Catalytic Reactions for Energy Storage with Transient Spectroscopy</b>	<b>272</b>
Tanja Cuk, Matthias Waeglele, Hoang Doan, Kevin Pollack, Xihan Chen, David Herlihy	
<b>Nanomaterials design for energy conversion and storage</b>	<b>273</b>
Yi Cui	
<b>Illuminating trap states of nanocrystalline titanium dioxide and their role in dye-sensitized solar energy conversion</b>	<b>274</b>
Fritz Knorr, Riley Rex, Jeanne McHale	
<b>Triboelectric Nanogenerator – a new energy technology using organic materials</b>	<b>276</b>
Zhong Lin Wang	
<b>Research on the multicomponent catalytic liquefaction technology of corn stalk features</b>	<b>277</b>
Li Xiangyu, Li Xueqin, Shi Junyou, Qi Wei	
<b>Effect of Co-doping with Trivalent Cations on the Dopant Local Structure, Optical Properties, and Exciton Dynamics in Cu(I)-doped ZnSe Quantum Dots</b>	<b>278</b>
Jin Zhang, Sheraz Gul, Jason Cooper	
<b>Polymer Materials for Energy Generation and Storage</b>	<b>281</b>

Zhenan Bao	
<b>Monodisperse Nanocrystals Crafted by Capitalizing on Amphiphilic Nonlinear Block Copolymers as Nanoreactors for Energy</b>	<b>282</b>
Zhiqun Lin, Xinchang Pang, Congshan Wan, Mengye Wang	
<b>Graphene-Semiconductor Composites for Photocatalytic and Photoelectrochemical Production of Fuels</b>	<b>283</b>
Nianqiang Wu, Fanke Meng	
<b>Catalytic conversion of glycerol and crude glycerol (by-product from bio-diesel industry) to oxygenated fuel additive with A continuous-flow process</b>	<b>284</b>
Malaya Nanda, Zhongshun Yuan, Wensheng Qin, Hassan Ghaziaskar, Marc-Andre Poirier, Chunbao (Charles) Xua	
<b>SOLVENT ISOTOPE EFFECT ON TRANSFER HYDROGENATION OF H<sub>2</sub>O with GLYCERINE UNDER ALKALINE HYDROTHERMAL CONDITIONS</b>	<b>286</b>
Zheng Shen, Wenjie Dong, Minyan Gu, Yalei Zhang, Fangming Jin	
<b>Developing near infrared semiconductor quantum dots and plasmonic nanostructures for solar cell applications</b>	<b>289</b>
Dongling Ma	
<b>Rational Nanostructure Designs for Energy Storage and Conversion</b>	<b>290</b>
Liangbing Hu	
<b>Role of nitrogen in catalysis and supporting nanoparticles on graphene</b>	<b>291</b>
Jianguo Wang, Xinde Wang, Xing Zhong	
<b>Nanocarbon Based Electrocatalysts for PEM Fuel Cells</b>	<b>293</b>
Yuehe Lin	
<b>Carbon Nanomaterials as Metal-free Catalysts for Energy Conversion</b>	<b>294</b>
Liming Dai	
<b>Semiconductor Nanowires for Energy Conversion</b>	<b>295</b>
Peidong Yang	
<b>Effect of carbon source and hydrogen source for formic acid formation under hydrothermal conditions with Mn</b>	<b>296</b>
Lingyun Lyu, Guodong Yao, Fangmin Jin, Jia Duo, Zhibao Huo	
<b>Chemical Looping Technology</b>	<b>298</b>
Liang-Shih Fan	
<b>Bifunctional Silver (I) Catalysis for CO<sub>2</sub> Upgrading</b>	<b>299</b>
Liang-Nian He, Qing-Wen Song	
<b>Catalytic CO<sub>2</sub> Activation and Hydrogenation Based on First Principles Computational Analysis</b>	<b>301</b>
Qingfeng Ge	
<b>A novel approach to CO<sub>2</sub> electroreduction based on 3D-Cu/Sn nanostructured</b>	<b>302</b>

<b>oxides related catalysts with high selectivity and stability</b>	
Jinli Qiao, Yuyu Liu, Jiujunn Zhang	
<b>Photocatalytic CO<sub>2</sub> Reduction with Water for Solar Fuel Production Using MgO-Modified TiO<sub>2</sub> Nanomaterials</b>	<b>304</b>
Lianjun Liu, Ying Li	
<b>Rapid and highly effective conversion of biomass and CO<sub>2</sub> into chemicals and fuels under hydrothermal conditions</b>	<b>305</b>
Fangming Jin, Zhibao Huo, Guodong Yao	
<b>Understanding Shape effect in catalysis: a case study of ceria nanoshapes as catalyst and catalyst support</b>	<b>307</b>
Zili Wu, Amanda Mann, Meijun Li, Steven Overbury	
<b>In-situ studies on the water gas shift reaction: From planar to powder catalysts</b>	<b>308</b>
Dario Stacchiola	
<b>Kinetics and mechanisms of C-C forming and C-O cleavage reactions of interests in bio-oil upgrading</b>	<b>309</b>
Daniel Resasco	
<b>A Commercial Demonstration of biorefinery of lipids---- Coproduction of Biodiesel and 1,3-propanediol</b>	<b>310</b>
Dehua Liu	
<b>Fundamental understanding of nanocatalytic materials for environmental protection and clean energy production</b>	<b>311</b>
Xianqin Wang	
<b>One-step synthesis of supported Pt-based electrocatalysts</b>	<b>312</b>
Xiulan Hu, Jianbo Zhang, Junjun Shi, Xiaodong Shen	
<b>Synthesis of highly photo-stable CuInS<sub>2</sub>/ZnS core shell quantum dots</b>	<b>314</b>
Liang Li	
<b>Three-dimensional Self-supported Electrocatalysts For Highly Efficient water splitting</b>	<b>315</b>
Shi Zhang Qiao, Sheng Chen	
<b>Recent progress in understanding the photocatalytic properties of bismuth vanadate</b>	<b>317</b>
Gyeong Hwang, Kyoung Kweon	
<b>Engineered doping to metal oxide nanorod arrays for improved photoelectrochemical water splitting activity</b>	<b>318</b>
Shaohua Shen	
<b>Understanding Semiconductor Water Interface for Improved Solar Water Splitting</b>	<b>319</b>
Dunwei Wang	
<b>Oxide Heteronanostructures for Solar Water-Splitting</b>	<b>320</b>



Lionel Vayssieres

- Oxygen-Deficient Metal Oxide Nanostructured Electrodes for Solar Hydrogen Generation** 321  
Yat Li
- An Ultimately Simple Synthetic Method for Spherical Mesoporous (Metal) Oxide Nanoparticles Using Supercritical Alcohols** 322  
Pengyu Wang, Kazuya Kobiro
- Hydrothermal Production of Aviation Fuels from Fatty Acid Esters and Microalgae Lipids** 324  
Jie Fu, Cuiyue Yang, Jianghua Wu, Zhaoyin Hou, Xiuyang Lu
- Surface Modified Spherical Activated Carbon Beads for Industrial CO<sub>2</sub> Capture Applications** 326  
Nannan Sun, Chenggong Sun, Hao Liu, Jingjing Liu, Trevor Drage, Colin Snape, Kaixi Li, Wei Wei
- Effects of Ce on Catalytic CO<sub>2</sub> Reforming of CH<sub>4</sub> over 5%Ni/ZSM-5** 327  
Mingchen Tang, Long Xu, Maohong Fan
- Multifunctional Polymer Gels for Advanced Energy and Environmental Applications** 329  
Guihua Yu
- Bio-mimetic functional hierarchical materials inspired from nature species** 330  
Di Zhang, Wang Zhang, Jiajun Gu, Shenming Zhu, Huilan Su, Qinglei Liu
- Charge transfer dynamics in multifunctional colloidal nanorod-metal tip heterostructures: H<sub>2</sub> generation and plasmon induced photochemistry** 331  
Tianquan Lian
- Cobalt-imbedded zeolite catalyst for direct synthesis of gasoline via Fischer-Tropsch synthesis** 332  
Yi Zhang
- Development of Hydrogenation Catalysts in Coal-derived Syngas to Ethanol Conversion Processes** 334  
Jihong Cheng, Wei Di, Yuan Liu, Shuxun Tian, Qi Sun
- What can pK<sub>a</sub> and NBO charges of the ligands tell us about the water and thermal stability of Metal Organic Frameworks?** 336  
Min Fang, Ping Lu, Yong Wu, Hong Kang, Haiyan Wei, Hongke Liu
- Technology development and deployment of clean coal conversion to fuels and chemicals in China** 339  
Yizhuo Han
- A potential technology with low energy cost in Ni smelting based on direct reduction of NiO to Ni with glucose under hydrothermal conditions** 340  
Guodong Yao, Zhibao Huo, Fangming Jin
- Hydrothermal conversion of carbon dioxide into methanol over copper** 342

Zhibao Huo, Jun Fu, Guodong Yao, Xu Zeng, Fangming Jin

**Particle size and crystal structure effects on pyrolysis behavior of iron sulfides in Argonne Premium Coals and a Maya petroleum vacuum resid asphaltene as examined with S-XANES** 344

Trudy Bolin

**Preparation of Higher Alcohol Synthesis Catalysts from Molybdenum Cluster Precursors** 347

Haiquan Su, Yulong Zhang, Na Wang, Xiaoman Wang

## 7. Advances in High Throughput Catalyst Development and Screening

**Exploration of the Role of Synthesis on Catalytic Performance of Cobalt-based Catalysts Guided by Factorial Designs** 348

Jason Hattrick-Simpers, Cun Wen, Jochen Lauterbach

**Impact of High Throughput Experimentation on Homogeneous Polyolefin Catalyst Research** 350

David Devore, Roxanne Jenkins

**Scanning Impedance Probe for High-Throughput Electrochemical Characterization of Solid State Electrodes** 351

Robert Usiskin, Shingo Maruyama, Chris Kucharczyk, Ichiro Takeuchi, Sossina Haile, Xiaohang Zhang

**Catalytic reactivity and electronic structure across continuous  $\text{Cu}_x\text{Pd}_{1-x}$  and  $\text{Cu}_x\text{Au}_y\text{Pd}_{1-x-y}$  composition space** 352

James Miller, Gamze Gumuslu, Chunrong Yin, Andrew Gellman

**High Throughput Screening of Model Supported Heterogeneous Catalysts using Thermography** 353

Brian Hayden, Jovine Emmanuel

**What we've learned from testing >250,000 Cells: New cell evaluation methods and data mining techniques** 355

Steven Kaye, David Brecht, Gang Cheng

**Oxidation of  $\text{Al}_x\text{Fe}_y\text{Ni}_{1-x-y}$  alloys across composition space** 356

Andrew Gellman, Mathew Payne, James Miller

## 8. 2nd International Symposium on Mesoporous Zeolites

**Mesoporous zeolites: an industrial view** 357

Carlo Perego, Roberto Millini

**Enhancement of Catalytic Activity and Control of Reaction Pathway for Hydrocarbon Reforming over Mesoporous Zeolites Supporting Metal Nanoparticles** 358

Kyungsu Na, Nathan Musselwhite, Xiaojun Cai, Selim Alayoglu, Gabor Somorjai

**Cost Reduction In The Production Of Mesostructured Zeolite For Fluid Catalytic Cracking** 361

Barry Speronello

<b>Textural Characterization of Catalytically Active Hierarchically Structured Zeolites via Gas Adsorption</b>	<b>363</b>
Katie Cychosz, Eric Li, Javier Garcia-Martinez, Matthias Thommes	
<b>Understanding Mesoporosity in Y Zeolite and its Application in Fluid Catalytic Cracking</b>	<b>364</b>
Shankhamala Kundu, Dieter Wallenstein, Wu-Cheng Cheng	
<b>Integrated Nanocatalysts with Mesoporous Silica Supports</b>	<b>366</b>
Hua Chun Zeng	
<b>Stabilization of ZnO in mesoporous ZSM-5 for methane dehydroaromatization</b>	<b>367</b>
Yungchieh Lai, Götz Vesper	
<b>Influence of the Si/Al ratio on H-ZSM-5 lattice and reaction site characteristics</b>	<b>369</b>
Susanne Opalka, Edward Schreiner, Raul Lobo, Rhonda Willigan, Tianli Zhu, Meredith Colket	
<b>Mesoporous Zeolites by Fluoride Route</b>	<b>371</b>
Valentin Valtchev, Zhengxing Qin	
<b>Synchronous adsorption of SO<sub>2</sub>, NO and CO<sub>2</sub> using modified zeolite assistant by the microwave irradiation</b>	<b>373</b>
Yinghui Han, Maohong Fan, Armistead Russell, Shuangchen Ma	
<b>Synthesis of ultra-large pore zeolites</b>	<b>376</b>
Fei-Jian Chen, Hong-Bin Du	
<b>Design of hierarchical micro-mesoporous materials for different catalytic applications using surfactant-mediated zeolite recrystallization</b>	<b>378</b>
Irina Ivanova	

## **9. Carbon dioxide Management: Recent Advances in Carbon dioxide Capture, Conversion, Utilization and Storage**

<b>Silicones for CO<sub>2</sub> Capture and EOR</b>	<b>380</b>
Robert Perry, Michael O'Brien, Mark Doherty, Benjamin Wood, Tiffany Westendorf, Robert Enick, Eric Beckman, Jason Lee, Stephen Cummings, Aman Dhuwe	
<b>Solid solution MOFs for CO<sub>2</sub> separation and regeneration with low energy consumption</b>	<b>382</b>
Satoshi Horike, Susumu Kitagawa	
<b>Metal coordination in salophen-linked covalent organic polymers for enhanced CO<sub>2</sub> capture</b>	<b>383</b>
Jeehye Byun, Damien Thirion, Cafer Yavuz	
<b>Metal-organic frameworks designed for carbon dioxide capture from flue gas</b>	<b>386</b>
Joseph Hupp	
<b>Identifying zeolite frameworks for enhanced CO<sub>2</sub> capture and separation applications</b>	<b>387</b>
Jeffrey Rimer, Radha Motkuri	

<b>Evaluating Transformational Solvent Systems For Post-Combustion CO<sub>2</sub> Separations</b>	<b>388</b>
David Heldebrant, Roger Rousseau, Vassiliki-Alexandra Glezakou, Phillip Koech, Feng Zheng, Mark Bearden, Charles Freeman	
<b>Carbon dioxide sorption in metal organic polyhedras at high pressure and high temperature</b>	<b>390</b>
Edson Perez, John Ferraris, Kenneth Balkus, Jr., Inga Musselman	
<b>Synthesis and Characterization of Multifunctional Porous Diazaborole-Linked Polymers</b>	<b>392</b>
Zafer Kahveci, Hani El-Kaderi	
<b>Direct air capture with amine functionalized porous polymer networks</b>	<b>393</b>
Hong-Cai Zhou, Weigang Lu	
<b>The strategies for improving carbon dioxide chemisorption by functionalized ionic liquids</b>	<b>394</b>
Sheng Dai	
<b>Ionic liquids for carbon capture</b>	<b>395</b>
De-en Jiang	
<b>Co-polymerization assisted synthesis of mesoporous carbonaceous adsorbents for efficient CO<sub>2</sub> capture</b>	<b>396</b>
Xiang Zhu, Tian Jin, Jun Hu, Honglai Liu, Sheng Dai	
<b>Critical Role of the Solvent in Promoting CO<sub>2</sub> Capture by Alkanolamines: A Theoretical Perspective.</b>	<b>397</b>
Dhivya Manogaran, Eunsu Paek, Haley Stowe, Gyeong Hwang	
<b>Novel liquid-like nanoparticle organic hybrid materials for CO<sub>2</sub> captrure and conversion</b>	<b>399</b>
Ah-Hyung Park, Camille Petit	
<b>Nanoporous Materials for Electrocatalytic CO<sub>2</sub> Reduction</b>	<b>401</b>
Feng Jiao	
<b>Effects of Oxygen Incorporation into CO<sub>2</sub>-derived Carbon Networks on Oxygen Reduction Reaction</b>	<b>402</b>
Jae Lee, Ayeong Byeon, Joonho Park, Yousung Jung	
<b>Electronchemical Reduction of CO<sub>2</sub> to Fuels using Supported Transition Metal Clusters: Comparison with Gas-phase Reactions</b>	<b>403</b>
Cong Liu, Peter Zapol, Larry Curtiss	
<b>Constructing Hybrid Photocatalysts for Efficient CO<sub>2</sub>-to-Fuel Conversion</b>	<b>405</b>
Tong Jin, Chao Liu, Michael Louis, Gonghu Li	
<b>Monodisperse Au Nanoparticles for Selective Electrocatalytic Reduction of Carbon Dioxide</b>	<b>407</b>
Shouheng Sun	

<b>Electroreduction of carbon dioxide on indium-based nanoparticles</b>	<b>408</b>
James White, Andrew Bocarsly	
<b>Visible Light Driven Reduction of CO<sub>2</sub> by Water on Modified Sr<sub>3</sub>Ti<sub>2</sub>O<sub>7</sub></b>	<b>410</b>
Balasubramanian Viswanathan	
<b>Ensemble Effects in Cu-alloy Catalysts for CO<sub>2</sub> Reduction</b>	<b>413</b>
Tim Mueller	
<b>Photoelectrochemical reduction of CO<sub>2</sub> on hybrid organic/inorganic photocathodes</b>	<b>415</b>
Csaba Janáky, Attila Kormányos, Hursán Dorottya, Krishnan Rajeshwar	
<b>The Role of Aqueous Phase Hydrogenation on CO<sub>2</sub> Capture and Conversion</b>	<b>416</b>
Hongfei Lin	
<b>DFT Studies on Facet Dependence of CO<sub>2</sub> Electroreduction Path and Selectivity</b>	<b>418</b>
Xiaowa Nie, Wenjia Luo, Michael Janik, Aravind Asthagiri	
<b>Hydrogenation CO<sub>2</sub> to formic acid over Ru supported on carbon nanotubes</b>	<b>420</b>
Na Liu, Xin He, An Zhou	
<b>Electrically promoted catalytic methane oxidative coupling with carbon dioxide over La-perovskite oxide catalysts</b>	<b>421</b>
Tomohiro Yabe, Kei Sugiura, Kazumasa Oshima, Shuhei Ogo, Yasushi Sekine	
<b>Vanadium-Potassium-Alumina catalyst: A way of promoting CO<sub>2</sub> and coke reaction in the presence of O<sub>2</sub> during the FCC catalyst regeneration</b>	<b>423</b>
Thiago da Silva, Rafael dos Santos, Nuno Batalha, Marcelo Pereira	
<b>Control of Physical Aging in Super Glassy Polymer Membranes Without Permeability Loss</b>	<b>426</b>
Matthew Hill, Cher Hon Lau, Phuc Tien Nguyen, Aaron Thornton, Kristina Konstas, Cara Doherty, Roger Mulder, Laure Bourgeois, Amelia Liu, David Sprouster, James Sullivan, Timothy Bastow, Anita Hill, Douglas Gin, Richard Noble	
<b>Rational design of oxide catalysts for carbon dioxide activation and hydrogenation</b>	<b>428</b>
Cynthia Lo, Zhuo Cheng	
<b>Mixed-Oxides for Carbonaceous Fuel Conversion with Integrated CO<sub>2</sub> Capture via Chemical Looping with Oxygen Uncoupling (CLOU)</b>	<b>430</b>
Fanxing Li, Nathan Galinsky, Arya Shafiefarhood	
<b>Artificial Photosynthesis Using Double Layered Hydroxides</b>	<b>432</b>
Kentaro Teramura, Shoji Iguchi, Hirotaka Ishii, Saburo Hosokawa, Tsunehiro Tanaka	
<b>Mechanism for Diffusion of CO<sub>2</sub> in Silica-Supported Amine Sorbents</b>	<b>433</b>
David Mebane, Kuijun Li	
<b>Thermosensitive Polyethylenimine for High Efficient Carbon Dioxide Release</b>	<b>435</b>

Johannes Kainz, Bernhard Rieger

**A polymeric membrane system for efficient CO<sub>2</sub> separation** **437**

Sung Gap Im, Youngmin Yoo, Kwanyong Pak, Ji Yeon Kim

**Assessment of CO<sub>2</sub>BOLs-PSAR for CO<sub>2</sub> Capture from Flue Gas based on Bench-Scale Testing Results** **439**

David Heldebrant, Paul Mathias, Feng Zheng, Mukund Bhakta, Mark Bearden, Charles Freeman, Andy Zwoster, Phillip Koech, Philip Jessop

**Fixation of CO<sub>2</sub> with concrete sludge** **441**

Akihiro Yamasaki, Miyuki Noguchi, Motoki Inoue, Atsushi Iizuka, Miyuki Takahashi

**Potential impact of combustion contaminants in saline formation** **442**

Yee Soong, Bret Howard, Sheila Hedges, Robert Dilmore

**CO<sub>2</sub> Release from Capture Solutions Using Nano-particles for Direct Solar-to-Thermal Conversion: Releasing CO<sub>2</sub> and lowering the specific heat penalty** **444**

Aaron Esser-Kahn, Du Nguyen, Samantha Goetz

**Ab initio Predictions of Carbon Dioxide Capture and Gas Separations using Metal-Organic Frameworks** **446**

Yousung Jung, Joonho Park, Heejin Kim

**Theoretical Synthesis of Mixed Solid Sorbents for CO<sub>2</sub> Capture Applications** **447**

Yuhua Duan, Dan Sorescu, David Luebke, Bryan Morreale, Xianfeng Wang, Bingyun Li, Keling Zhang, Xiaohong Li, David King

**Absorption characteristics of CO<sub>2</sub> based on 1-(4-butylamino)-3-methyl imidazolium chloride ionic liquids** **450**

Yi Zhao, Lijuan Yang, Wei Sun, Huining Xiao, Qiangwei Li

**Small associative thickeners for supercritical CO<sub>2</sub>** **460**

Robert Enick, Jason Lee, Eric Beckman, Stephen Cummings, Robert Perry, Michael O'Brien, Mark Doherty

**Capture of CO<sub>2</sub> by [NH<sub>2</sub>p-mim]Br Ionic Liquid** **462**

Qiangwei Li, Yi Zhao, Lidong Wang, Lijuan Yang

**Identifying molecular mechanisms for CO<sub>2</sub> capture by aqueous amines using first principles-based atomistic modeling** **464**

Haley Stowe, Eunsu Paek, Dhivya Manogaran, Gyeong Hwang

## **10. Batteries and Fuel Cell Technologies: Challenges and Solutions towards Global Stewardship**

**In Situ Formed Si Nanoparticle Network with Micron-Sized Si Particles for Lithium-Ion Battery Anodes** **466**

Mingyan Wu, Wen Yuan, Sang-Jae Park, Vincent Battaglia, Gao Liu

**Advanced Biner Design in High Capacity Silicon Anodes of Lithium Ion Batteries** **468**

You Kyeong Jeong, Tae-woo Kwon, Ali Coskun, Jang Wook Choi

**Sum frequency generation in tandem with cyclic-voltammetry: Unveiling the solid electrolyte interface chemistry on Si anodes and Au cathodes** **469**

Yonatan Horowitz, Fei-Fei Shi, Phil Ross, Gabor Somorjai

**Temperature effect of electrochemical performance in Li-ion battery with silicon anodes** **470**

Wen Yuan, Hui Zhao, Vincent Battaglia, Gao Liu

**Three dimensional Si/SiO<sub>x</sub>-C nanocomposite as anode materials for lithium-ion battery** **471**

Sang Hyun Cho, Sungho Park, Jung Hyuk Moon, In Sub Jung

**In situ characterization of Li transport in Li<sub>x</sub>Sny anodes with neutrons** **473**

Anne Co, Danny Liu, Jinghui Wang, Marcello Canova, Lei Cao

**Si Nanotubes ALD Coated with TiO<sub>2</sub>, TiN or Al<sub>2</sub>O<sub>3</sub> as High Performance Lithium Ion Battery Anodes** **475**

David Mitlin

**Insights into Electrochemical Properties of Amorphous TiO<sub>2</sub> for Application in High Power Lithium-ion Batteries** **477**

Haitao Fang, Bingmei Feng, Dongsheng Guan, Huixin Wang, Xue Sun

**Structure and Conductivity of Liquid Crystals having Carbonate Units for the Use as Electrolytes in Lithium-Ion Batteries** **480**

Andreas Eisele, Konstantinos Kyriakos, Christine Papadakis, Bernhard Rieger

**Advances in Electrolytes for Lithium Ion Batteries: A Mechanistic Understanding** **482**

Brett Lucht, Mengqing Xu, Cao Cuong Nguyen

**Graphene supported mesoporous single crystals silicon on Cu foam as stable lithium-ion battery anode materials** **483**

Hao Jiang, Chunzhong Li, Shilong Jing

**Surface Reconstruction and Chemical Evolution of Stoichiometric Layered Cathode Materials for Lithium-Ion Batteries** **484**

Feng Lin, Isaac Markus, Dennis Nordlund, Tsu-Chien Weng, Mark Asta, Huolin Xin, Marca Doeff

**In-situ ATR-FTIR investigation of the solid electrolyte interface (SEI) on single-crystal Si anodes for Li ion batteries** **486**

Feifei Shi, Kyriakos Komvopoulos, Philip Ross, Gabor Somorjai

**Use of complimentary methods to evaluate energy storage interfaces** **487**

Eric Dufek, Lucia Petkovic, Harry Rollins, John Klaehn

**Investigations of Solid Electrolyte Interphase Formation on High-Capacity Li-ion Battery Anodes** **488**

Zhenzhen Yang, Michael Thackeray, Lynn Trahey

**Challenges in Development of High-Fidelity, Physics-Based, Lithium-Ion Battery Models** **490**

Rajeswari Chandrasekaran, Chulheung Bae, Yeonkyeong Seong, Theodore Miller

**A high-performance aromatic carbonyl-based organic cathode for sodium-ion batteries** **492**

Wei Luo, Xiulei Ji

**Electrode-electrolyte solution interactions between TiO<sub>2</sub> nanotube electrode and nonaqueous electrolytes for sodium-ion batteries** **493**

Hui (Claire) Xiong, Richard Cutler, Riley Parrish, Ganesh Kamath, Subramanian Sankaranarayanan

**Sodium Secondary Batteries with Amide Ionic Liquids** **495**

Toshiyuki Nohira, Rika Hagiwara, Kazuhiko Matsumoto, Changsheng Ding, Chen Chih-Yao, Takayuki Yamamoto, Koma Numata, Atsushi Fukunaga, Shoichiro Sakai, Koji Nitta

**High-capacity anode materials for sodium ion batteries** **496**

Youngjin Kim, Yong Il Kim, Seung Mo Oh, Kyu Tae Lee

**The Emergence of Na-ion Battery Technologies** **498**

Christopher Johnson, Sanja Tepavcevic, Hui Xiong, Tijana Rajh

**Anodes for Sodium Ion Batteries based on Tin - Germanium - Antimony Alloys** **500**

David Mitlin

**Positive impacts of defects and amorphous nature of electrodes for Li-ion and Na-ion batteries** **502**

Guozhong Cao

**Imidazole Containing Hyperbranched Perfluorinated Polymer Blends Towards Anhydrous Proton Exchange Membranes** **503**

Matthew Quast, Aaron Argall, Anja Mueller

**Thin film catalysts for PEMFCs** **505**

Vladimir Matolin, Roman Fiala, Michal Vaclavu, Iva Matolinova

**Sustainability assessment of regenerative hydrogen fuel cells for energy storage** **506**

Matthew Pellow, Christopher Emmott, Sally Benson

**The origin and mechanism of Pt/C cathode catalyst degradation in polymer electrolyte fuel cell by anode gas exchange cycles studied by in situ time-resolved XAFS** **509**

Kotaro Higashi, Gabor Samjeske, Shinobu Takao, Shin-ichi Nagamatsu, Kensaku Nagasawa, Oki Sekizawa, Takuma Kaneko, Tomoya Uruga, Yasuhiro Iwasawa

**Enabling fuel versatility in polymer electrolyte fuel cells with state of the art anion exchange membranes and/or novel molecular catalysts** **510**

Andrew Herring, Vinh Nguyen, Quanning Li, Rajeswari Janarthanan, Lauren Greenlee, Madhura Joglekar, Brian Trewyn

**Low Platinum Loaded Graphene Based Electrode Layers for PEM Fuel Cell** **512**

Lale Işıkeli Şanlı, Begüm Yazar, Vildan Bayram, Selmiye Alkan Gürsel

**Modified Proton Exchange Membranes for Fuel Cells Operating at Elevated Temperature and Low Humidity** **514**

Sangaraju Shanmugam



<b>Dissimilar oxide interfaces to accelerate oxygen reduction kinetics</b>	<b>516</b>
Bilge Yildiz, Yan Chen, Nikolai Tsvetkov	
<b>Nanostructured or fine grained doped ceria ceramics</b>	<b>517</b>
Mojka Otonicar, Noemí Walsöe de Reca	
<b>Supercapacitor based on metallic nanowires as electrodes for power integrated circuits</b>	<b>518</b>
Daniel Choi	
<b>High-Performance Lithium-Sulfur Battery: From Molecular Understanding to Nanomaterials Design</b>	<b>519</b>
Weiyang Li, Zhi Wei Seh, Guangyuan Zheng, Qianfan Zhang, Hongbin Yao, Yi Cui, Yuan Yang	
<b>The Quest for Batteries with a Sulfur Cathode: Will Nano-membranes Impact their Viability</b>	<b>521</b>
Claudiu Bucur, John Muldoon	
<b>Iron embedded Carbon fiber derived by Silk fibroin and Ketjenblack composite Electrocatalyst for Cable-type flexible Zinc-air battery</b>	<b>522</b>
Joohyuk Park, Jaephil Cho	
<b>Quantifying rechargeability limitations in Li-O<sub>2</sub> batteries</b>	<b>523</b>
Bryan McCloskey	
<b>IMPROVING THE PERFORMANCE OF LITHIUM-SULFUR BATTERIES USING CONDUCTIVE POLYMER AND MICROMETRIC SULFUR POWDER</b>	<b>524</b>
Zihui Wang, Yulin Chen, Vincent Battaglia, Gao Liu	
<b>Nanomaterials design for batteries</b>	<b>526</b>
Yi Cui	
<b>Pyrolysis of cellulose under ammonia leads to nitrogen-doped nanoporous carbon generated through methane formation</b>	<b>527</b>
Xiulei Ji, wei luo	
<b>Insights into nanoscale phase stability and charging mechanisms in alkali-O<sub>2</sub> batteries from first principles calculations</b>	<b>529</b>
Shyue Ping Ong, ShinYoung Kang, Yifei Mo, Gerbrand Ceder	
<b>All-solid-state lithium batteries using Ti-based cathode materials and sulfide solid electrolyte</b>	<b>532</b>
Yoon Seok Jung, Bum Ryong Shin, Young Jin Nam, Jin Wook Kim	
<b>Polymer-based batteries: From organic radical batteries (ORBs) to redox flow batteries (RFBs)</b>	<b>534</b>
Ulrich Schubert, Tobias Janoschka, Bernhard Haeupler, Thomas Jaehnert, Andreas Wild, Daniel Schmidt, Rene Burges, Martin Hager	
<b>Nanostructured V<sub>2</sub>O<sub>5</sub>/Sn Mg-ion Full Batteries</b>	<b>536</b>
Sanja Tepavcevic, Tijana Rajh, Dehua Zhou, Christopher Johnson	
<b>How to Develop Ultra-Long Life Energy Storage</b>	<b>538</b>

Ping Liu

**Tailoring Lithium-Intercalation Host Structure for Rechargeable Magnesium Ion Cathodes** **539**

Yan Yao, Yanliang Liang, Yifei Li, Hyun Deog Yoo

**11. Challenges and Opportunities in Petroleum Oil Production, Refining and Utilization**

**Crystal microbalance investigation of the corrosion of common alloying elements in oil with naphthenic acid** **540**

Brian Patrick, Rajashree Chakravarti, Thomas Devine

**Development of a new catalytic method to substantially reduce high temperature naphthenic corrosion in the refinery** **542**

Rajashree Chakravarti, Brian Patrick, Thomas Devine

**Generation of H<sub>2</sub>S by Crude Fractions at High Temperature** **544**

Peng Jin, Gheorghe Bota, Srdjan Nesic, Fernando Farelas, Winston Robbins

**Evaluation of Scales Protective Properties in Naphthenic Acid Challenges** **546**

Gheorghe Bota

**Modeling of internal corrosion of pipelines in oil/gas production** **548**

Frank Cheng

**Effect of Machine Hammer Peening Surface Treatment on Pitting Corrosion Behavior of Oil-Grade Alloy 718** **549**

Ting Chen

**CORROSION INHIBITION IN HIGHLY AGGRESSIVE SOLUTIONS** **553**

G. Burstein, B. Daymond, V. Choda

**In-situ studies of crude oil stability and direct visualization of asphaltenes aggregation processes via some spectroscopy techniques** **554**

Oleg Martyanov, Evgeniy Morozov, Sergey Trukhan, Velu Subramani, Sergey Kazarian, Yuriy Larichev, Anton Gabrienko

**ASPHALTENE DEPOSITION AND REMOVAL** **555**

Seyma Aslan, Abbas Firoozabadi

**Upgrading oilsands bitumen: Solvent deasphalting and visbreaking sequence** **556**

Ashley Zachariah, Arno de Klerk

**Oxidative ring-opening over metal oxides** **558**

Natalia Montoya Sánchez, Arno de Klerk

**Inorganics Driven High Temperature Fouling of Metal Surfaces in Oil Refining** **562**

David Mitlin

**Asphaltene Solubility and Fouling** **564**

Estrella Rogel, Cesar Ovalles, Michael Moir

<b>Reduction of Crude Overhead Corrosion Through Changes in Unit Operating Philosophy</b>	<b>567</b>
Brandon Payne, Collin Cross	
<b>Aggregation of Model Asphaltene in Heptol Investigated by Molecular Dynamics Studies</b>	<b>570</b>
Cuiying Jian, Tian Tang	
<b>Oxidation of naphthenic-aromatic compounds in bitumen</b>	<b>572</b>
Muhammad Siddiquee, Arno de Klerk	
<b>Study of Phase Behavior for Some Sugar-based Surfactants and Their Applications in Enhanced Oil Recovery by Chemical Flooding</b>	<b>575</b>
Yongfu Wu, Frances Fournier, Susanna Toivonen, Scott Rosencrance	
<b>Viscosity of hydrocarbons at high temperatures and pressures</b>	<b>579</b>
Robert Enick, Hseen Baled, Peter Koronaios, Randy Miles, Ma Luo, Ward Burgess, Yee Soong, Isaac Gamwo, Deepak Tapriyal, Mark McHugh, Yue Wu, Babatunde Bamgbade	
<b>Coal liquefaction liquid quality: Impact of temperature and iron pyrite</b>	<b>581</b>
Ioan-Tudor Apan, Arno De Klerk	
<b>Ionic Liquids as Viscosity Modifiers for Heavy Oils</b>	<b>583</b>
Deepa Subramanian, Kathleen Wu, Abbas Firoozabadi	
<b>Analysis of pyrolysis products of latex gloves by gas chromatography mass spectrometry (GC-MS)</b>	<b>584</b>
Nasrollah Hamidi, Sujana Shrestha, Marketa Marcanikova, Sihon Chang, Louis Whitesides, Ruhullah Massoudi	
<b>DFT Analysis of Steric Interactions in Models of Unstable Petroleum Constituents</b>	<b>586</b>
Peter Seidl	
<b>Fractionation by solvent blends and characterization by NMR of asphaltenes from colombian crude oils</b>	<b>587</b>
Fernanda Silva, Lina Navarro, Peter Seidl, Maria José Guimarães, Kátia Leal	
<b>FUNCTIONALIZED CARBON NANOTUBES FOR ADSORPTIVE DESULFURIZATION OF MODEL FUEL OILS</b>	<b>589</b>
Mohammad Siddiqui, Tawfik Saleh, Basheer Chabasha	
 <b>12. 10th International Symposium on Hydrotreating and Hydrocracking Technologies</b>	
<b>Opportunities and challenges in hydrotreating sour fuel gas</b>	<b>591</b>
Henrik Mortensen	
<b>State of the art testing of refining catalysts</b>	<b>593</b>
Sascha Vukojevic, Alfred Haas, Jochen Berg, Florian Huber, Marius Kirchmann, Tilman Sauer	
<b>Effect of 1,2-Cyclohexanediamine-N,N, N', N'-Tetraacetic Acid as complexing agent in a Hydrodesulfurization NiWS/Al<sub>2</sub>O<sub>3</sub> catalyst</b>	<b>594</b>

Carlos Santolalla-Vargas, Victor Suarez-Toriello, Jorge Chavarria, Jose de los Reyes, Barbara Pawelec, Jose Luis Fierro

**Unsupported NiMoS catalysts prepared from emulsions formed by ultrasonic irradiation** **596**

Luis Lippolis, Héctor Guzmán, Carmelo Boívar, Pedro Pereira-Almao, Carlos Scott

**Asphaltenes Hydroprocessing** **599**

Fernanda Isquierdo, Carlos Scott, Gerardo Vitale, Pedro Almao

**NiWS hydrocracking catalysts: Imaging WS<sub>2</sub> slabs 2D morphology and improving their sulfidation via a new method.** **601**

Thibault Alphanz, Diane Bijou, Maria Girleanu, Audrey Bonduelle-Skrzypczak, Christèle Legens, Pascal Raybaud, Christophe Coperet, Anne-Sophie Gay, Ovidiu Ersen

**Hydrocracking of 1-methylnaphthalene catalyzed by zeolite-alumina composite supported NiMo catalysts** **604**

Atsushi Ishihara

### **13. Production, Distribution and Utilization of Dimethyl Ether as a Transportation Fuel**

**Process design for the KOGAS' one-step synthesis of DME** **606**

Taekyong Song, Wonjun Cho, Young-soon Baek, Okbae Kwon, Hyenchan Lee, Yong-gi Mo

**Kinetic study of low and intermediate temperature oxidation of dimethyl ether** **608**

Brian Brumfield, Naoki Kurimoto, Xueliang Yang, Pascal Dievert, Joseph Lefkowitz, Gerard Wysocki, Yiguang Ju, Tomoya Wada

**Numerical simulation of high pressure dimethyl ether (dme) injection under diesel engine conditions** **611**

Khanh Cung, Seong-Young Lee, Jaclyn Johnson, Sreenath Gupta, Gregory Siuchta

**Nanoparticle emissions from dimethyl ether combustion in a compression ignition engine** **613**

William Northrop, Kathleen Vignali, David Kittelson

**Emissions and Performance Benchmarking of a Prototype Dimethyl Ether-Fueled Heavy-Duty Truck** **614**

James Szybist, Samuel McLaughlin, Suresh Iyer

**HISTORICAL PERSPECTIVE, STATUS AND FUTURE PROMISE OF DME AS AN ADVANCED FUEL** **616**

Theo Fleisch

**High Efficiency Combustion with DME and Propane Fumigation into Diesel Engine Intake Air** **617**

Bhaskar Prabhakar, Andre Boehman

**An Investigation of Injection and Combustion of Dimethylether Using High Pressure Injection System** **619**

Masaaki Kato, Takamasa Yokota, Jost Weber, Mitsuru Konno, Ernst Winklhofer, Karl Wieser, Herwig

Ofner, Denis Gill

**DME Combustion in Heavy Duty Diesel Engines** 621

Ingemar Denbratt, Henrik Salsing

**Small-scale Production to Develop Regional Markets: Launching DME Fuel in North America** 623

Elliot Hicks

## **14. Applications of X-Ray and Neutron Scattering Techniques in Energy Technologies**

**Development and application of Al EXAFS to characterize Al T-sites in zeolite: effect of hot liquid water treatment on the HBEA zeolite framework** 625

Aleksei Vjunov, John Fulton, Donald Camaioni, Mirosław Derewinski, Johannes Lercher

**Investigation of supported catalysts for C-H bond activation by X-ray spectroscopic techniques** 627

Andrew Getsoian, Bo Hu, Neil Schweitzer, Guanghui Zhang, Ujjal Das, Peter Stair, Adam Hock, HackSung Kim, Jeffrey Miller

**Bond strains and reactivity of supported metal nanocatalysts** 629

Anatoly Frenkel

**Dehydration effect on pore size, porosity, specific surface area and fractal parameters of shale rocks: USAXS study** 632

Sungwon Lee, Robert Klingler, Jan Ilavsky, Randall Winans, Timothy Fischer, Douglas McCarty, Marcus Wigand

**In Situ X-ray Studies of Subnanometer and Nanometer Size Cluster-Based Catalysts** 634

Stefan Vajda

**In Situ X-ray Scattering Studies of High Temperature and Pressure Catalysis for High Performance Scram Jet Engines** 636

Kamila Wiaderek, Sungsik Lee, Sungwon Lee, Mrunmayi Kumbhalkar, James Dumesic, Randall Winans

**Study of PFSA ionomers using x-ray scattering techniques** 638

Ahmet Kusoglu, Adam Weber

**Using insitu SAXS to elucidate phase separated morphology and dynamics in next generation ionomers for polymer membrane based electrochemical energy conversion devices** 639

Andrew Herring, Ashley Maes, Yuan Liu, Soenke Seifert, Feilong Liu, Daniel Knauss, E. Coughlin, S. Ertem

**Potential Dependent Structures at Pt(111) Electrode/Electrolyte Interfaces Studied by in situ Surface X-ray Scattering** 641

Toshihiro Kondo, Takuya Masuda, Nana Aoki, Kohei Uosaki

**Visualizing water in non-precious metal catalyst-based polymer electrolyte fuel cells using neutron imaging** 642

Rangachary Mukundan, Dusan Spornjak, Gang Wu, Daniel Hussey, David Jacobson, Andrew Steinbach, Rodney Borup, Piotr Zelenay

- X-ray and Neutron Studies of the Structure, Dynamics, and Transport Properties of Polyelectrolytes for Energy Applications** **645**  
Kirt Page, Christopher Soles, Christopher Stafford
- X-ray scattering and absorption studies of polymer electrolyte fuel cell cathode electrocatalysts** **646**  
Nancy Kariuki, Deborah Myers, James Gilbert
- In Situ Small-Angle Neutron Scattering Studies of Battery Electrodes** **648**  
Craig Bridges, Xiao-Guang Sun, Jinkui Zhao, M. Parans Paranthaman, Sheng Dai, William Heller
- Applications of synchrotron x-ray and neutron techniques in battery material research** **649**  
Yang Ren, Bachir Aoun, Zonghai Chen
- Multiscale Neutron and X-Ray Tomographic Studies on High Capacity Lithium Battery Chemistries** **650**  
Jagjit Nanda, Hassina Bilheux, Yijin Liu, Joy Andrews, Sreekanth Pannala, Kenneth Herwig
- Tetragonal vs. cubic phase stability in Al – free Ta doped  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  Garnet Li Ion Solid Electrolyte** **652**  
Travis Thompson, Jeff Wolfenstine, Jan Allen, Michelle Johannes, Ashfia Huq, Jeff Sakamoto
- From atoms to electrodes: Mesoscale effects in electrochemical conversion** **654**  
Olaf Borkiewicz, Kamila Wiaderek, Nathalie Pereira, Glenn Amatucci, Peter Chupas, Karena Chapman
- Monitoring mobile ions: X-ray and neutron diffraction studies of emerging battery materials** **656**  
Peter Khalifah, Jue Liu, Xiao-Qing Yang, Ashfia Huq, Pamela Whitfield, Mikhail Feygenson, Joerg Neufeind, Jianming Bai
- Unveiling molecular level detail of  $\text{CO}_2$  adsorption in several extensive families of Metal-Organic Frameworks** **657**  
Wendy Queen, Craig Brown, Matthew Hudson, Eric Bloch, Jeffrey Long, Jarad Mason, Miguel Gonzalez, Jason Lee
- Neutron scattering studies of adsorbates in metal-organic frameworks** **659**  
Craig Brown
- In Situ X-ray Scattering and Microscopy of Energy Materials Processing and Operation** **661**  
Michael Toney
- Neutron radiography of fluid flow for energy research** **663**  
Lawrence Anovitz, Phillip Bingham, Yarom Polsky, Justin Carmichael, Hassina Bilheux, David Jacobson, Daniel Hussey, Lawrence Anovitz, Phillip Bingham, Yarom Polsky, Justin Carmichael, Hassina Bilheux, David Jacobson, Daniel Hussey, Lawrence Anovitz, Phill
- Combined Neutron and High-Resolution Electron Microscopy Study of Particle Fracture in Lithium Manganospinel  $\text{LiMn}_2\text{O}_4$**  **664**

Bart Bartlett, Xiaoguang Hao

**X-ray Nano-imaging Application on Energy Materials** 667

Jun Wang

## **15. Applications of Theoretical Chemistry for Energy and Fuel Production**

**Hydrogen trapping potential of titanium functionalized Mg-BN-framework** 668

Madhu Samolia, T. J. Kumar

**Predictions of rate constants for hydrogen abstraction reactions by resonantly-stabilized free radicals** 669

Kun Wang, Stephanie Villano, Anthony Dean

**Oxidation of Chlorobenzene using Au-, Au/Pd- and Pd-ZSM-5 Zeolite Catalysts: A DFT Study** 671

Bundet Boekfa, Masahiro Ehara, Hidehiro Sakurai, Thana Maihom, Jumras Limtrakul

**Frontier orbital interpretation of gas release pathways in lignin thermolysis** 675

Preetinder Virk, Michael Klein

**Modeling of 2-Bromotrifluoropropene Flame Inhibition** 678

Donald Burgess, Jeffrey Manion, Valerie Babushok, Gregory Linteris

**DFT study of the mixed aldol condensation reaction catalyzed by acidic Zeolites HZSM-5 and HY** 680

Angela Miguez, S. Vaitheeswaran, Scott Auerbach

**A layered Manganese oxide as a bifunctional material for capturing sunlight and catalyzing water splitting: Theory and Simulation** 681

Jose Mendoza-Cortes, William Goddard III

**Interface controlled growth of Ceria Nanoarrays on Anatase Titania Powder** 682

Hyun You Kim, Ping Liu, Mark Hybertsen

**Effect of Surface Defects on Electronic and Optical Properties of Silicon Quantum Dots** 684

Naveen Dandu, Svetlana Kilina, Dmitri Kilin

**Excited States, Spectroscopy, and Energy Conversion in Organic Semiconductors from First Principles** 685

Jeffrey Neaton

**Ferroelectric oxides for visible-light photovoltaics and engineering of shift current** 686

Feng Gong Wang, Fan Zheng, Ilya Grinberg, Hiroyuki Takenaka, Andrew Rappe

**Near-infrared Light Driven Photocatalytic Water Splitting** 688

Jinlong Yang

**Multiscale QM/MM simulation of catalytic reactions and redox processes for solar fuels** 689

Weitao Yang

- The Harvard Clean Energy Project – a virtual high-throughput search framework for new organic solar cell materials** **690**  
Johannes Hachmann, Edward Pyzer-Knapp, Alan Aspuru-Guzik
- Vertical and Lateral Phase Segregations of Organic Solar Cells from Device-Level Coarse-Grained Molecular Simulations** **691**  
Chun-Wei Pao
- Neural network potentials for large-scale molecular dynamics simulations of condensed systems** **693**  
Jörg Behler
- DFT+U calculations of rare earth CeO<sub>2</sub> for catalysis and energy production** **695**  
Xueqing Gong, Jie Zhang, Ya-Ling Song, Xin-Ping Wu, Fendy Chen, Peijun Hu, Guanzhong Lu
- Novel materials for alkane dehydrogenation: A systematic study on Pt based, subnanometer-sized alloy cluster catalysts** **696**  
Andreas Hauser, Martin Head-Gordon, Alexis Bell
- The catalytic capacity of a Cr-phthalocyanine porous sheet** **698**  
Qiang Sun
- Computational Study of Aqueous Phase Phenol Hydrogenation over Metal Catalysts** **699**  
Yeohoon Yoon, Roger Rousseau, Robert Weber, Johannes Lercher, Donghai Mei
- DFT studies of biomass conversion catalyzed by acidic zeolites** **702**  
Subramanian Vaitheeswaran
- A Key Player for Designing Novel Energy-Related Materials: Multi-Scale Simulation Based on First-Principles and Reactive Force Field** **710**  
Sang Soo Han
- Mechanisms for heterogeneous and homogeneous reduction of carbon dioxide from first principles** **712**  
Emily Carter
- Electronic energy level alignment at the water interface of a model oxide and nitride photoelectrode** **713**  
Michiel Sprik, Andrew Meng, Jun Cheng
- First-Principles Modeling Approach Towards Quinone-Derivatives for Li ion battery: Effect of Molecular Architecture on Electrochemical Properties** **714**  
Ki Chul Kim, Seung Woo Lee, Seung Soon Jang
- First principles descriptors for identifying molecular co-catalysts that facilitate efficient electroreductions for renewable energy** **715**  
John Keith
- Kinetic Theory for Stability of Supported Metal Particles Under Reaction Conditions** **717**



Sulei Hu, Runhai Ouyang, Wei-Xue Li	
<b>Graphene supported clusters for hydrogen storage and electrocatalysis</b>	<b>718</b>
Qingfeng Ge	
<b>Computational Study of Silicon Nanocrystals for Energy and Optoelectronic Applications</b>	<b>719</b>
JUN-WEI Luo	
<b>Stochastic GW: Formulation and application to nanoclusters</b>	<b>721</b>
Christopher Arntsen, Daniel Neuhauser, Yi Gao, Eran Rabani, Roi Baer, Cyrus Karshenas	
<b>Ab initio calculations of charge transports in nanosystems</b>	<b>722</b>
Lin-Wang Wang	
<b>Multi-scale simulations of functional materials</b>	<b>723</b>
Youyong Li	
<b>Theoretical study of the effect of the length of silicon nanowires on the band gap</b>	<b>724</b>
Walid Hassan, Amit Verma, Reza Nekovei, Mahmoud Khader, M. Anantram	
<b>Calculating electron-phonon couplings to evaluate the charge and thermoelectric transports in organic and carbon materials</b>	<b>726</b>
Zhigang Shuai	
<b>Design, Synthesis, and Characterization of Organic Sensitizers with Cascade Energy Levels for Long-Lived Charge Separated States</b>	<b>728</b>
Lichang Wang, Xueqin Zhou, Dongzhi Liu, Wei Li, Tianyang Wang, Krishanthi Weerasinghe	
<b>Computational design of 3<sup>rd</sup> generation electron donating polymers for organic photovoltaic solar cells</b>	<b>729</b>
Yongwoo Shin, Jaikai Liu, Xi Lin	
<b>Electronically non-adiabatic dynamics in singlet fission: a quasi-classical trajectory simulation</b>	<b>730</b>
Guohua Tao	
<b>Exciton Dynamics in Disordered Molecular Environments</b>	<b>731</b>
Adam Willard	
<b>Excited State Dynamics in Light Harvesting Materials</b>	<b>732</b>
John Parkhill	
<b>Discovery of nanoporous materials for energy applications</b>	<b>734</b>
Maciej Haranczyk, Richard Martin, Cory Simon, Berend Smit	
<b>TOWARD RAPID PREDICTIONS OF GAS ADSORPTION AND DIFFUSIVITY IN NANOPOROUS MATERIALS</b>	<b>735</b>
Jianzhong Wu	
<b>Molecular simulations of ternary alkane-water-surfactant mixtures with two or three liquid phases</b>	<b>736</b>
J. Ilja Siepmann, David Harwood, Angel Cortes-Morales, Cornelis Peters, Peng Bai	

<b>Unified charge transfer associated strain destabilization mechanism of hydrogen clusters around bcc metal vacancies</b>	<b>738</b>
Xing-Qiu Chen Chen, Weiwei Xing	
<b>Computational screening of metal-organic frameworks for hydrogen and natural gas storage</b>	<b>740</b>
Diego Gomez-Gualdron, Bhaskarjyoti Borah, Hongda Zhang, Yamil Colon, Randall Snurr	
<b>Sensitivity of Chemical Pathways in Reactive Networks</b>	<b>741</b>
Rex Skodje, Michael Davis, Zeb Kramer, Weixue Li, Shirong Bai, Xiang Kui Gu	
<b>First-principles Study of NO Oxidation Kinetics on Low Index LaCoO<sub>3</sub> Perovskite Surfaces</b>	<b>742</b>
Xiao Liu, Zhengzheng Chen, Yanwei Wen, Rong Chen, Bin Shan	
<b>New approach to detailed kinetic modeling for hydrocarbon pyrolysis from fundamental quantum-chemical principles</b>	<b>744</b>
Mikhail Ryazantsev, Adeel Jamal, Keiji Morokuma	

## **16. Energy and Fuels Storch Award in Fuel Science: Symposium in Honor of Professor S. Ted Oyama**

<b>Can nickel phosphides become viable hydroprocessing catalysts?</b>	<b>745</b>
Stuart Soled, Sal Miseo, Joseph Baumgartner, Javier Guzman, Trudy Bolin, Randall Meyer	
<b>Combined in situ XAFS and FTIR study of Ni phosphide catalysts</b>	<b>746</b>
Kyoko Bando, Takahiro Wada, Satoru Takakusagi, Shigeo Oyama, Kiyotaka Asakura	
<b>Kinetic and Spectroscopic Studies of Catalytic Mechanisms: Hydrodeoxygenation of Biomass Feedstocks on Transition Metal Phosphides</b>	<b>747</b>
Ted Oyama, Ayako Iino, Jeun Shin, Phuong Bui, Ara Cho, Atsushi Takagaki, Ryuji Kikuchi, Kyoko Bando	
<b>Low temperature steam reforming of ethanol over PtNi/CeO<sub>2</sub>-nanocube catalyst</b>	<b>749</b>
Tamara Moraes, Raimundo Rabelo-Neto, Mauro Ribeiro, Lisiane Mattos, Marios Kourtelesis, Spyros Ladas, Xenophan Verykios, Fabio Noronha	
<b>CO-free hydrogen production using low temperature ethanol steam reforming</b>	<b>750</b>
Armando Borgna, Catherine Choong, Yonghua Du, Martin Schreyer, Luwei Chen	
<b>Distinctive coordination chemistry of chromium chlorides responsible for the superior catalytic performance in glucose conversion in ionic liquids</b>	<b>752</b>
Huixiang Li, Tingyu Huang, Wenjuan Xu, Zhanwei Xu, Z. Conrad Zhang	

## **17. Advances in Analytical Methods for Petroleum Upstream Applications**

<b>Ambient Analysis of Nitrogen compounds in Petroleum Oil using Desorption Atmospheric Pressure Chemical Ionization</b>	<b>753</b>
Fred Jjunju, Simon Maher, Anyin Li, Hsu-Chen Hsu, Stephen Taylor, R. Graham Cooks	
<b>Thermal Crackability of Oils and Their Derived Fractions</b>	<b>756</b>

Lante Carbognani, Estrella Rogel, Josune Carbognani, Cesar Ovalles, Francisco Lopez-Linares, Pedro Pererira-Alamo

**APGC/MS for characterization of the Macondo wellhead crude oil and the oil spill 760**

Vladislav Lobodin, Ryan Rodgers, Alan Marshall

**Method for Rapid Evaluation of Additives to Prevent Asphaltene Precipitation at Reservoir Temperatures 762**

Cesar Ovalles, Estrella Rogel, Harris Morazan, Michael Moir

**Crude Oils Analysis by ICP-OES and ICP-MS via direct dilution 765**

Francisco Lopez-Linares, Jenny Nelson, Laura Nannini, David Leong, Lidia Berhane

**$^1\text{H}$  AND  $^{13}\text{C}$  NMR characterization of oil shale crude at various process stages of distillate fuel production 767**

J Bays, David King, James Franz, Thomas Gallant, Molly O'Hagan, John Linehan, James Patten, James Bunger

**Comparing Asphaltenes: Deposit versus Crude Oil 769**

Estrella Rogel, Michael Roye, Toni Miao

**Optimization of Mass Range, Dynamic Range, Signal-to-Noise Ratio, Mass Resolution, and Mass Accuracy for Characterization of Petroleum by FT-ICR Mass Spectrometry 772**

Alan Marshall, Greg Blakney, Tong Chen, Yu Chen, Christopher Hendrickson, Nathan Kaiser, Daniel McIntosh, Amy McKenna, John Quinn, Ryan Rodgers, Chad Weisbrod

**Investigation of the hydrolyzed polyacrylamide/metal complexes gel chemistry through NMR 774**

Teresa Lehmann, Vladimir Alvarado, Elena Topchiy

**Advances in Gas Chromatography for Sulfur Analysis in Petroleum Upstream, Downstream and Petrochemical Applications 776**

Carl Rechsteiner, John Crandall, Ned Roques

**Analytical methods for various in-field measurements of methane and arsenic in hydraulic fracturing operations 777**

Jack Driscoll, Jennifer Maclachlan

## **18. Fischer-Tropsch Chemistry and Catalysis**

**Fischer-Tropsch Synthesis: Activity and selectivity of  $\chi\text{-Fe}_5\text{C}_2$  and  $\Theta\text{-Fe}_3\text{C}$  carbides 779**

Muthu Kumaran Gnanamani, Dennis Sparks, Robert Keogh, Burtron Davis, Hussein Hamdeh, Wilson Shafer, Gary Jacobs

**Principles of olefin selectivity in Fischer-Tropsch synthesis on iron- and cobalt catalysts 781**

Hans Schulz

**Novel utilization of mesostructured cellular silica foams as support of cobalt catalysts in Fischer-Tropsch synthesis 783**

Liang Wei, Yuhua Zhang, Yanxi Zhao, Chengchao Liu, Jinlin Li, Jingping Hong	
<b>Effect of tube diameter on the radial temperature gradient of a pilot-scale fixed-bed reactor for iron-based Fischer-Tropsch synthesis</b>	<b>788</b>
Nonam Park, Jeong-Rang Kim, Yeonshick Yoo, Jinsuk Lee, Myung-June Park	
<b>Effect of ZnAl<sub>2</sub>O<sub>4</sub> morphologies on the catalytic performance of Co-based catalysts in Fischer-Tropsch Synthesis</b>	<b>791</b>
Junkun Yan, Ming Wu, Jingping Hong, Yuhua Zhang, Jinlin Li	
<b>Influence of promoters on physico-chemical properties and performance of Co-MWCNTs catalyst for Fischer-Tropsch Synthesis</b>	<b>795</b>
Vahid Vosoughi, Ajay Dalai, Nicholas Abatzoglou	
<b>Fischer Tropsch synthesis: Enhanced selectivity to n-alcohols and olefins over transition metal oxide doped ceria supported cobalt catalysts</b>	<b>797</b>
Mauro Ribeiro, Muthu Gnanamani, Israel Azevedo, Raimundo Rabelo-Neto, Ramana Pendyala, Gary Jacobs, Burtron Davis, Fabio Noronha	
<b>Factors influencing the design of a Fixed Bed Fischer-Tropsch Reactor</b>	<b>800</b>
Rafael Espinoza	
<b>CO Activation on HCP and FCC Cobalt Catalysts</b>	<b>801</b>
Wei-Xue Li, Jinxun Liu, Haiyan Su	
<b>Evidence of highly active Co oxide catalyst for the Fisher-Tropsch Synthesis</b>	<b>803</b>
Gerome Melaet, Walter Ralston, Gabor Somorjai, Selim Alayoglu	
<b>CoMn carbon supported catalysts for Fischer Tropsch synthesis</b>	<b>804</b>
SARWAT IQBAL, Stuart Taylor, Graham Hutchings, Thomas Davies, Khalid Karim	
<b>Surface Reactivity of Iron and Iron Carbides in CO Hydrogenation</b>	<b>806</b>
M Ozbek, J Niemantsverdriet	
<b>Commercializing an advanced Fischer-Tropsch synthesis technology</b>	<b>809</b>
Stephen LeViness, Heinz Robota, Soumitra Deshmukh, Amanda Miller, Thomas Yuschak, Matthew Davis	
<b>Effects of halogenated acids and hydrogen cyanide in syngas on a precipitated iron Fischer-Tropsch synthesis catalyst</b>	<b>813</b>
Wenping Ma, Gary Jacobs, Dennis Sparks, Burtron Davis	
<b>Impact of sulfur on a Co/Mn based catalyst for syngas conversion to olefins</b>	<b>816</b>
Jia Yang, John Walmsley, Bjorn Enger, Torbjorn Gjervan, Svatopluk Chytil, Rune Myrstad, Magnus Ronning, De Chen, Asad Khan, Khalid Karim	
<b>Fischer-Tropsch Synthesis: High Oxygenate Selectivity of Hydrothermal Carbon Supported Cobalt Catalysts</b>	<b>818</b>
Uschi Graham, Gary Jacobs, Muthu Gnanamani, Stephen Lipka, Wilson Shafer, Christopher Swartz, Burtron Davis	
<b>Inverse and normal isotope effects during iron catalyzed Fischer-Tropsch synthesis</b>	<b>821</b>

Buchang Shi, Yunxin Liao

**Small-scale gas-to-liquids using Fischer–Tropsch synthesis: Opportunity or myth?** 823

Arno de Klerk

**Fischer-Tropsch mechanism: Studies of a Co/Ce<sub>0.75</sub>Si<sub>0.25</sub> catalyst using <sup>13</sup>C<sup>18</sup>O** 825

Debanjan Chakrabarti, Muthu Gnanamani, Wilson Shafer, Dennis Sparks, Vinay Prasad, Arno De Klerk, Burtron Davis, Mauro Ribeiro

**Fischer-Tropsch synthesis over high-loading Co-based catalysts in a microreactor** 828

Anders Holmen, Jia Yang, Sara Eiras, Rune Myrstad, Peter Pfeifer, Hilde Venvik

**Effects of surfactants on the performance of Co nano-particles for Fischer-Tropsch synthesis** 831

FENG GUO, Botao Teng

**3-D characterization of Fischer-Tropsch catalysts before and after reduction** 832

Ilke Arslan, Sanchita Dey, John Roehling, Joost Batenburg, Burtron Davis

**Characterization of nano-scale Pt promoted yttria-stabilized zirconia catalysts for hydrogen production applications** 833

Michela Martinelli, Gary Jacobs, Luca Lietti, Carlo Visconti, Shelley Hopps, Burtron Davis

**Assessing the impact of promoter spatial distribution in Mn-promoted Co FTS catalysts using novel STEM-EDS quantitative methods** 835

Gregory Johnson, Sebastian Werner, Alexis Bell

**Improving the accessibility of Fischer-Tropsch catalyst layers by insertion of transport pores** 837

Henning Becker, Robert Güttel, Thomas Turek

**Conversion of Syngas to Higher Alcohols: Influence of bentonite clay as a binder and its variable loading in KCoRhMoS<sub>2</sub>/MWCNT catalysts formulation** 841

Philip Boahene, Ramaswami Sammynaiken, Ajay Dalai

**The effects of intracrystalline diffusion and aromatization of hexane at various pressures using isotopic labeling** 842

Wilson Shafer, Gary Jacobs, Gabriela Alvez, Ryan Snell, Xianghong Hao, Burtron Davis

## **19. Mesoporous and Nanostructured Hybrid Materials: Symposium in Honor of Prof. Thomas J. Pinnavaia**

**Enhancing the stability of copper chromite catalysts for the selective hydrogenation of furfural using ALD overcoating** 844

Christopher Marshall, Hongbo Zhang, A. Jeremy Kropf, Guanghui Zhang, Jeffery Elam, Jeffery Miller, Fred Sollberger, Fabio Ribeiro, Eric Stach, James Dumesic

**Mesoporous catalytic materials for biomass valorization to fuels and chemicals** 846

Konstantinos Triantafyllidis

## **20. Advances in Chemistry of Energy and Fuels**

<b>Hydrogenation of furfural to butanol and pentanols for renewable gasoline blendstocks</b>	<b>848</b>
Kristi Fjare, Yun Bao	
<b>Characteristics of Zn, Cu and As in fast pyrolysis residues of different particle size of sewage sludge</b>	<b>850</b>
Hongmei Jin, Zhizhou Chang, Renato Arazo, Sergio Capareda	
<b>Effects of HCl on the oxidation of CH<sub>4</sub> over CeO<sub>2</sub></b>	<b>856</b>
Li-Li Yin, Xue-Qing Gong	
<b>Ambient hydrolysis deposition of TiO<sub>2</sub> in nanoporous carbon and the converted TiN-carbon capacitive electrode</b>	<b>857</b>
Xingfeng Wang, Vadivukarasi Raju, Wei Luo, Bao Wang, William Stickle, Xiulei Ji	
<b>Reactivity of hydrogen controlled by oxygen vacancies at CeO<sub>2</sub>(111)</b>	<b>858</b>
Xin-Ping Wu, Xue-Qing Gong	
<b>Scalable fabrication of high surface area graphene from GO by magnesiothermic reaction</b>	<b>859</b>
Zhenyu Xing, Bao Wang, Xiulei (David) Ji	
<b>Renewable fuel additives from depolymerized lignin</b>	<b>860</b>
Heather Parker, Christopher Chuck, Matthew Jones, Joshua Spellman	
<b>Capture of CO<sub>2</sub> by 1-butyl-3-methylimidazole glycine ionic liquid under normal pressure</b>	<b>864</b>
Qiangwei Li, Yi Zhao, Lidong Wang, Lijuan Yang	
<b>Control of plasmonic nanoparticle dispersion in bulk heterojunction organic solar cells and consequences on active layer nanostructure</b>	<b>866</b>
Dennis Butcher, Lawrence Drummy, Hilmar Koerner, Frank Scheltens, David McComb, Robert Wadams, Laura Fabris, Christopher Bailey, Christopher Tabor, Michael Durstock	
<b>Analysis of Mercury Content in Petroleum Products</b>	<b>868</b>
Basheer Chanbasha	
<b>Effect of Dipole Moment on Dye-Sensitized Solar Cells</b>	<b>874</b>
Boyang Chu, Hong Wang, Ka-Ho Lee, Tingbin Yang, Zilong Wang, Zhenyang Lin, Yongye Liang, Jianwei Sun, Shihe Yang	
<b>Multiple ambient hydrolysis deposition of tin oxide into nanoporous carbon as a stable anode for Lithium-ion batteries</b>	<b>878</b>
Vadivukarasi Raju, Xingfeng Wang, Wei Luo, Xiulei Ji	
<b>Photoinduced charge transfer in the organic photovoltaic solar cells</b>	<b>880</b>
Yongwoo Shin, Xi Lin	
<b>Tuning the structure and gas sorption properties of metal-organic frameworks for hydrogen and methane storage</b>	<b>881</b>
Farshid Ramezanipour, Jeffrey Long, Miguel Gonzalez	

<b>Influence of surface modified with methanol under ultraviolet radiation on flotability of the macerals in Shenfu coal</b>	<b>882</b>
Zhao Wei, Zhou Anning	
<b>Towards a Cost efficient Production of Fuels from lignocellulosic Biomass using Ionic Liquids</b>	<b>883</b>
Florence Gschwend, Jason Hallett, Paul Fennell	
<b>Synthesis of Cobalt Disulfide on Reduced Graphene Oxide for Hydrogen Evolution Reaction</b>	<b>884</b>
Jieun Yang, Seongjoon Ahn, Hyeon Suk Shin	
<b>Synthesis of nanoporous 1,2,4-Oxadiazoles with high CO<sub>2</sub> capture capacity</b>	<b>886</b>
Dong Ah Ko, Hasmukh Patel, Cafer Yavuz	
<b>Iron fluoride hydrate/graphene nanocomposites as cathode materials for sodium secondary battery applications</b>	<b>888</b>
Ghulam Ali, Ji Young Kim, Kyung Yoon Chung	
<b>Electrochemical Performance of Ni-rich Layered Oxide LiNi<sub>0.8</sub>Co<sub>0.15</sub>Al<sub>0.05</sub>O<sub>2</sub> Cathode Material by Surface Modification using Organic Compound for Lithium Secondary Batteries</b>	<b>889</b>
Dong Hyun Kim, Ji Young Kim, Kyung Yoon Kyung Yoon	
<b>A Study on Cr-based anode material of sodium batteries</b>	<b>890</b>
SE YOUNG KIM, Kyung Yoon Chung	
<b>Engineering of Templated Protein Assembly for Elucidation of High-Performance Oxygen Reduction Reaction: Surfactant-Free Gold-Platinum Bimetallic Nanoclusters on SWNT-Protein Assembly</b>	<b>891</b>
Yong-Tae Kim, Ji Hun Kim, Yong Ho Kim	
<b>Measuring Thermal Transport Properties of rGO Thin Film</b>	<b>892</b>
A-Rang Jang, Dongwoo Kang, Hyeon Suk Shin	
<b>Comparative study of rutile SnO<sub>2</sub> (110) and TiO<sub>2</sub> (110) for formic acid adsorption and decomposition</b>	<b>894</b>
Miru Tang, Qingfeng Ge	
<b>Non Syn-Gas Catalytic Route to Methanol Production</b>	<b>895</b>
Fenglin Liao, Cheng-Tar Wu, Edman Tsang	
<b>Electron Transportation Mechanism of Conductive Polymer Binder for Si anode in Lithium Battery</b>	<b>896</b>
Guo Ai, Wen Yuan, Yulin Chen, Hui Zhao, Sang Park, Gao Liu	
<b>Effect of oxygen on acetic acid steam reforming</b>	<b>898</b>
Vissanu Meeyoo, Thirasak Rirksomboon, Nat Phongpreuksathatb, Atsadang Traiangwongb	
<b>Materials modelling for energy and fuels: From photovoltaics to photocatalysis</b>	<b>900</b>
Taizo Shibuya, Kenji Yasuoka, Susanne Mirbt, Biplab Sanyal, Lee Burton, Jonathan Skelton, Aron Walsh	

<b>Enhanced Sulfur Tolerance of the Samarium (Sm)-doped Cerium oxide (CeO<sub>2</sub>): A First-Principles Study</b>	<b>901</b>
Dong-Hee Lim, Sangheon Lee, Hee Su Kim, Sung Pil Yoon, Jonghee Han, Suk Woo Nam, Chang Won Yoon, Hyung Chul Ham	
<b>Cobalt doped TiO<sub>2</sub> anatase (100) surface photoelectrochemical cell: Computational spin restricted analysis of surface ingrained vs. above surface models</b>	<b>903</b>
Stephanie Jensen, Dmitri Kilin	
<b>Role of Solvation on Electron Dynamics of Titanium Hydroxide</b>	<b>904</b>
Dayton Vogel, Dmitri Kilin	
<b>Size-dependent chemistry in gasoline direct injection (GDI) particulate matter</b>	<b>905</b>
Samuel Lewis, John Storey	
<b>Hierarchy benefits the SCR-DeNO<sub>x</sub> activity of V<sub>2</sub>O<sub>5</sub>/TiO<sub>2</sub> mixed oxide catalysts</b>	<b>906</b>
Erisa Saraci, Robert Arndt, Jens Kullmann, Dirk Enke, Roger Gläser	
<b>Modified Sn surfaces for the electrochemical reduction of CO<sub>2</sub></b>	<b>908</b>
Jeremy Feaster, Etosha Cave, Toru Hatsukade, David Abram, Kendra Kuhl, Chris Hahn, Thomas Jaramillo	
<b>High voltage energy storage systems using facile patterning approach</b>	<b>909</b>
Inho Nam, Gil-Pyo Kim, Soomin Park, Joeng Woo Han, Seongjun Bae, Sungju Yu, Ha Nee Umh, Su Young Lee, Yong Hwa Kim, jongheop Yi	
<b>Plasmon-enhanced solar energy conversion to chemical and electrical energy</b>	<b>910</b>
Sungju Yu, Yong Kim, Su Young Lee, Hyeon Don Song, Ha Nee Umh, Jongheop Yi	
<b>Production of valuable chemicals (1,3-butadiene) from biomass-based resources alternative to the petroleum</b>	<b>911</b>
Jayeon Baek, Tae Yong Kim, Inho Nam, Soomin Park, Sungju Yu, Seongjun Bae, Su Young Lee, Ha Nee Umh, Yong Hwa Kim, Jongheop Yi	
<b>Characteristic of bismuth-antimony-tellurium thermoelectric materials via ultrasonic spray pyrolysis</b>	<b>912</b>
Hye Young Koo, Gook Hyun Ha, Kyung Tae Kim	
<b>Study on processing of metal foam via slurry coating</b>	<b>913</b>
Dahee Park, Eun-Mi Jung, Jung-Yeul Yun	
<b>Structures and Energetics of Carbon Dioxide Hydration over Copper Alkoxide Functionalization in Metal-Organic Frameworks: A DFT Study</b>	<b>914</b>
Chadchalem Raksakoon, Thana Maihom, Bundet Boekfa, Jumras Limtrakul	
<b>Comparison of CeO<sub>2</sub>/C supported Pt or Au catalysts activities towards ethylene glycol oxidation</b>	<b>917</b>
Virginija Kepeniene, Jurate Vaiciuniene, Rokas Kondrotas, Vidas Pakstas, Loreta Tamasauskaite Tamasiunaite, Eugenijus Norkus	
<b>Probability of trivalent molybdenum (d<sup>3</sup>) spin crossover in hexagonal phase NaYF<sub>4</sub> nanocrystals</b>	<b>918</b>



Ge Yao, Mary Berry, P. May, Dmitri Kilin

**Flexible Wwre-like all-carbon supercapacitors based on porous core-shell carbon fibers** **920**

Weijia Zhou, Xiaojun Liu, Kai Zhou, Shaowei Chen

**Charge-tunable polyampholytes for the enhanced flocculation of cellular biomass** **922**

Kathryn Morrissey, Chunlin He, Rebecca Chapman, Lucjan Żołnierowski, Shana Bender, William Prevatt, Mark Stoykovich

**Excited state non-adiabatic dynamics simulation of Ru cluster interfacing anatase TiO<sub>2</sub>(101) Surface and liquid water** **923**

Shuping Huang, Talgat M. Inerbaev, Dmitri S. Kilin

**Kinetic study and pyrolysis of lignite coal** **925**

Mehran Heydari, Moshfiqur Rahman, Rajender Gupta

**Ink-Jet Printing of Efficient Organic Solar Cells** **928**

Navid Attarzadeh, Reza Foudazi, Abbas Ghassemi

**ACTIVATED CARBON/NANOPARTICLES FOR ADSORPTIVE DESULFURIZATION OF MODEL FUEL OIL** **929**

Khalid Alhooshani