



255TH AMERICAN CHEMICAL SOCIETY
NATIONAL MEETING AND EXPOSITION

Nexus of

FOOD ENERGY & WATER.

NEW ORLEANS
LOUISIANA

MARCH 2018
18 — 22

PROGRAM BOOK



Peter K. Dorhout, Ph.D.
ACS President

PRESIDENTIAL SYMPOSIA AND EVENTS

SPONSORED AND RECOMMENDED BY THE ACS PRESIDENT

SATURDAY, MARCH 17, 2018

Presidential Outreach Event: Exploring Our World Through Chemistry

Cosponsored by CCA

Lyons Recreation Center

624 Louisiana Ave, New Orleans

10:00 AM - 1:00 PM

SUNDAY, MARCH 18, 2018

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clear Water

Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, INOR, I&EC, MPPG, SCHB & YCC

Hilton New Orleans Riverside | Grand Salon B
Sections 9/12 | First Floor

8:30 AM - 10:50 AM

Science Cafes and Engaging the Public: Techniques for Hosting Successful Events

Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, INOR, I&EC, MPPG, SCHB & YCC

Hilton New Orleans Riverside

Grand Salon B | Sections 9/12 | First Floor

1:30 PM - 5:20 PM

Nexus of Food, Energy, & Water

Sponsored by MPPG and Cosponsored by PRES

Ernest N. Morial Convention Center

Great Hall A First Floor

3:00 PM - 6:00 PM

MONDAY, MARCH 20, 2018

Community Sharing of Chemical Safety Data: Yes, No, Maybe?

Sponsored by CINF and Cosponsored by PRES
CA & CHAS

New Orleans Marriott Convention Center

River Bend 1 | Second Floor

8:20 AM - 12:20 PM

TUESDAY, MARCH 20, 2018

GSSPC: Finding Our Place at the Bottom: A Symposium in Memory of Richard Feynman

Sponsored by CHED and Cosponsored by PRES,
ANYL, COLL, ENVR, INOR & PMSE

New Orleans Marriott Convention Center

Blaine Kern C | First Floor

1:30 PM - 4:55 PM

OTHER SYMPOSIA RECOMMENDED BY THE ACS PRESIDENT

SUNDAY, MARCH 18, 2018

Science of Sexual Harassment

Sponsored by WCC and Cosponsored by PRES,
C&EN, PROF & YCC

Hilton New Orleans Riverside | Grand Salon C
Section 13 | First Floor

9:00 AM - 4:50 PM

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF and Cosponsored by PRES,
ANYL, BIOT, BIOL, CHED, CMA, COLL, COMP,
CWD, ENVR, INOR, MEDI, ORGN, PHYS, POLY,
PMSE, WCC & YCC

Hilton New Orleans Riverside

Grand Salon D Section 22 | First Floor

9:00 AM - 4:50 PM

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present

Scholar Research Symposium

CHED, DAC, MPPG & Louisiana Local Section

Hilton New Orleans Riverside | Grand Salon D
Section 24 | First Floor

1:00 PM - 4:40 PM

MONDAY, MARCH 19, 2018

State-of-the-Art: Two Decades Advancing the 12 Principles of Green Chemistry

Sponsored by CHED and Cosponsored by PRES
New Orleans Marriott Convention Center |

Blaine Kern E | First Floor

8:30 AM - 3:50 PM

Excellence in Graduate Polymer Research

Sponsored POLY and Cosponsored by PRES, PROF,
SOCED & YCC

New Orleans Marriott Canal Street | Studio 5
Second Floor

8:00 AM - 4:40 PM

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present

Sponsored by HIST and Cosponsored by PRES,
AGFD, CHED, DAC, MPPG & Louisiana Local Section

Hilton New Orleans Riverside | Grand Salon D
Section 24 | First Floor

8:30 AM - 5:40 PM

Information Legacy of Eugene Garfield: From the Chicken Coop to the World Wide Web

Sponsored by CINF and Cosponsored by
PRES & HIST

New Orleans Marriott Convention Center | River
Bend 1 | Second Floor

1:15 PM - 5:05 PM

Science of Sexual Harassment

Sponsored by WCC and Cosponsored by PRES,
C&EN, PROF & YCC

Hilton New Orleans Riverside | Grand Salon C
Section 13 | First Floor

3:00 PM - 5:00 PM

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Sponsored by PROF and Cosponsored by PRES,
ANYL, BIOT, BIOL, CHED, CMA, COLL, COMP,
CWD, ENVR, INOR, MEDI, ORGN, PHYS, POLY,
PMSE, WCC & YCC

Hilton New Orleans Riverside | Grand Salon D
Section 22 | First Floor

3:00 PM - 5:00 PM

TUESDAY, MARCH 20, 2018

Excellence in Graduate Polymer Research

Sponsored POLY and Cosponsored by PRES, PROF,
SOCED & YCC

New Orleans Marriott Canal Street | Studio 5
Second Floor

8:00 AM - 5:40 PM

Ernest N. Morial Convention Center | Hall D

First Floor

6:00 PM - 8:00 PM

Water Supply Safety

Sponsored by CHAS and Cosponsored by PRES,
CCS & ENVR

Hilton New Orleans Riverside | Grand Salon D
Section 21

First Floor

9:00 AM - 11:30 AM

Science Cafés and Engaging the Public: Techniques for Hosting Successful Events

Cosponsored by CATL, CELL, CHAS, CHED, COLL,
CPRC, CTA, ENVR, INOR, I&EC, MPPG, SCHB &
YCC

Hilton New Orleans Riverside

Grand Salon B | Sections 9/12 | First Floor

1:30 PM - 5:20 PM



PMSE 155: Self-assembly approach in halloysite nanotube composites

Authors

Rawil Fakhrullin (/acsnola2018/speaker/ab26580ed028519d8644fd7eec23f8a9)

Yuri M Lvov (/acsnola2018/speaker/1646715dad62c25eb44d3d6093c225f6)

Vladimir Vinokurov (/acsnola2018/speaker/ee74ac71b5ae2e339b8e7e82bb09c2c2)

Body

Yuri M Lvov^{2 1}, Vladimir Vinokurov¹, Rawil Fakhrullin³

1. Colloid Phys Chemistry, I. Gubkin Russian State University of Oil and Gas, Moscow, Russian Federation
2. Inst. for Micromanufacturing, Louisiana Tech University, Ruston, Louisiana, United States
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Halloysite micropatterning: Similar to nematic liquid crystals ordering, halloysite nanotubes can orient themselves along a common axis. The accumulation of tubes from an isotropic centre to the circumference increases the tubes concentration beyond a critical one governed by Onsager's theory for orientation of highly charged nanorods. The alignment is enhanced by higher concentrations, temperature, higher surface charge and length of the tubes. Such o-called "coffee ring" effect for halloysites was extended in applications for forming periodic rings along the length of glass capillary tube and micropatterns onto solid supports as was first demonstrated by M. Liu. Another application is drying of halloysite aqueous dispersion dropped onto small metal balls. Halloysites self-assemble into concentric barriers with periodicity of 0.1-0.2 mm and height of 2-5 mkm. One can use systematically place balls which confine the drying allowing for designed halloysite micropatterns, reminding interference of waves. Such micropatterns allowed for selective adsorption of aligned fibroblast cells along the nanotubes' orientation.

Self-assembly on biological surfaces: Halloysite self-assembly may be linked to surface irregularities with positioning driven by capillary forces and final fixation in dry state; it found an interesting applications in halloysite hair coating. When hair is exposed for aqueous halloysite dispersion and then dried, one is getting stable 4-5 mkm thick multilayer nanotube coating.

Pickering emulsion for spill oil bioremediation and catalysis: Halloysites can also assemble on an oil-water interface. Halloysites, both pristine and with surface hydrophobization, form oil-water Pickering microemulsions. Clay nanotubes positioned laterally on the oil-water interface are reducing the surface tensions and stabilizing the emulsion droplets. Pickering microemulsions with halloysite may be used in biphasic catalysis and spill petroleum bioremediation. The petroleum/water interface is roughened and microorganisms (*Alcanivorax borkumensis*, alkanotrophic bacteria widely distributed in marine environments) added for oil degradation are better attached to such oil droplets.

Sessions



PMSE 155: Self-assembly approach in halloysite nanotube composites

Monday, Mar 19 9:30 AM

Studio 9, New Orleans Marriott Canal Street

(/acsnola2018/event/1ad8094c93e26b609b420b33634ac6ef)

1:30 CATL 451. Photocatalytic oxidation of water soluble organic and pharmaceutical compounds using visible/near uv light. **R.D. Barreto**, M. Howell

1:50 CATL 452. Investigation of a facile, scalable synthesis route for bismuth oxychloride 2D nanostructures for photocatalytic water treatment. M. Robinson, S. Padilla, A. Pattammattel, L. Gómez-Velázquez, M. Bizarro Sordo, **V. Leppert**

2:10 CATL 453. Synthesis and application of a sustainable N-doped TiO₂/CdS nanohybrid composite for photocatalytic degradation of 4-chlorophenol. **A. Aragon**, W. Kierulff-Vieira, T. Lecki, M. Skompska, J. Widera

2:30 Intermission.

2:45 CATL 454. Solar-light driven photocatalytic degradation of organic pollutants using natural dye-sensitized TiO₂. **M. Ghosh**, A. Ray

3:05 CATL 455. Improvement of photoelectrochemical activity of ZnO/TiO₂ core-shell nanostructure through Ag nanoparticle integration. **Z. Wang**, X. Wang

3:25 CATL 456. Oxygen-doped nanoporous carbon nitride via water-based homogeneous supramolecular assembly for photocatalytic hydrogen evolution. **Z. Jingwen**, J. Zou, L. Pan

Innovative Chemistry & Materials for Electrochemical Energy Storage

Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

THURSDAY MORNING

Section A
Hampton Inn & Suites Convention Center
Antonine

Elucidation of Mechanisms & Kinetics on Surfaces
Cosponsored by COLL, ENVR and PHYS
L. Baker, S. Laursen, *Organizers*
A. Savara, *Organizer, Presiding*

9:00 CATL 457. Kinetic consequences of carbon and oxygen coverages during CO_x methanation and CH₄ dry reforming on Ni, Co, and Ni-Co clusters. **P.T. Lachkov**, Y. Chin

9:20 CATL 458. Investigating alkene formation pathways in methanol-to-hydrocarbon processes within zeolites. **P. Kravchenko**, M. Deluca, D. Hibbits

9:40 CATL 459. On the role of surface adsorbed oxygen in ethanol reaction pathways on Mo₂C. **C.A. Farberow**, C. Nash, J. Hall, J. Schaidle

10:00 CATL 460. Nature of the active sites for carbon dioxide reduction on metal nanoparticles: suggestions for optimizing performance. **T. Cheng**, Z. Wang, W.A. Goddard

10:20 Intermission.

10:40 CATL 461. Understanding activity loss in precious-metal combustion catalysts using well-defined nanocrystals. **E.D. Goodman**, A. Riscoe, N. Tahsini, F. Abild-Pedersen, A.C. Johnston-Peck, M. Cargnello

11:00 CATL 462. Kinetics modeling enabled parameterization and

discrimination of nanoparticle surface reactivity evaluated by chemical assays. **X. Bi**, P.K. Westerhoff

11:20 CATL 463. Early-stage catalytic behavior of ethane dehydroaromatization over zinc modified HZSM-5 catalyst via transient kinetic methods. **Y. Xiang**

Section B
Hampton Inn & Suites Convention Center
Riverside I

Unconventional Catalysis Targeting Stable Molecules

Cosponsored by ENFL, ENVR, INOR and PHYS
C. Wang, *Organizer*
C.L. Marshall, *Organizer, Presiding*
C. Wang, *Presiding*

9:00 CATL 464. Biomimetic oxidation catalyst from polymer-nanocrystal composite material. **A. Riscoe**, C. Wrasman, A. Hoffman, A. Menon, A. Boubnov, E. Goodman, S.R. Bare, M. Cargnello

9:20 CATL 465. Conversion of light alkanes to alkyl esters and chlorides using iodine oxides and chlorides: Radical versus non-radical pathways. **T.B. Gunnoe**, J.T. Groves, W.A. Goddard, N. Schwartz, N. Boaz, S.E. Kalman, G. Fortman, R. Fu, R.J. Nielsen, J.M. Goldberg

10:00 CATL 466. Electrochemical carbon dioxide conversion to alcohols. **F. Jiao**

10:40 Intermission.

10:50 CATL 467. Computational searches for energetically efficient CO₂ reduction reaction steps across chemical and materials space. M. Groenenboom, K. Saravanan, Y. Basdogan, **J.A. Keith**

11:30 CATL 468. Highly efficient functionalized porous UiO-66 based metal organic frameworks (UiO66-MOFs) as catalysts for cross coupling reactions. **P. Elumalai**, S.T. Madrahimov

Section C
Hampton Inn & Suites Convention Center
Riverside III

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels

Cosponsored by ENFL, ENVR and INOR
J. Choi, O. Gazit, M. Kidder, *Organizers*
A. Lepore, *Presiding*

9:00 CATL 469. Catalytic conversion of lignocellulosic feedstock to hydrocarbon fuel intermediates. **A. Padmaperuma**, M. Lilga

9:20 CATL 470. Computational study of aerobic oxidation of 4-(Hydroxymethyl)phenol (4-HMP) by Co(salen). **V. Nziko**, R.C. Johnston, A. Ivanov, T.J. Elder, A. Rudie, D. Turpin, S. Alam, J.J. Bozell, J.M. Parks

9:40 CATL 471. Withdrawn

10:00 CATL 472. Insights into glucosidic bond activation by paired metal chlorides in ionic liquid. **Y. Yang**, Z. Zhang, H. Li, P. Yan

10:20 Intermission.

10:40 CATL 473. Catalytic influence of naturally occurring salts on biomass

pyrolysis chemistry: A combined experimental and DFT study. **J.S. Arora**, K. Ansari, P.J. Dauenhauer, S. Mushrif

11:00 CATL 474. Hydrodeoxygenation reaction network of furylmethane oxygenates to jet and diesel range fuels: Probing the role of supported palladium catalyst and hafnium triflate promoter. **S. Dutta**, B. Saha, D.G. Vlachos

11:20 CATL 475. Catalytic conversion of natural cotton fibers to carbon nanotubes and nitrogen functionalization. **G. Zhao**, F. Gao, K. Li, Z. Wang, M. Jahan

Section D
Hampton Inn & Suites Convention Center
Bienville

General Catalysis

A. Savara, *Organizer*
M. Dixit, *Presiding*

8:00 CATL 476. Stereoinversion of R-configured secondary alcohols using a single enzymatic approach. **M.M. Musa**, I. Karume, M. Takahashi, S.M. Hamdan

8:20 CATL 477. Extremely fast olefin metathesis in aqueous media with 3rd generation Grubbs-type catalysts. A. Ashcraft, S. Balof, C. Jones, **H.J. Schanz**

8:40 CATL 478. Investigating the oxygen reduction reaction on inorganic/organic interfaces. **M. Anand**, S. Siahrostami, J.K. Norskov

9:00 CATL 479. Novel copper N-tosyl nitrenes from bis(pyrazolyl)methane ligands: Investigation of their reactivity towards catalysis. **J. Moegling**, A. Hoffmann, N. Orth, B. Venderbosch, R. Rampmeier, I. Ivanovic-Burmazovic, M. Tromp, S. Herres-Pawlis

9:20 CATL 480. Withdrawn

9:40 Intermission.

10:00 CATL 481. Transition metal nitrides for oxygen electrocatalysis. **H. Abroshan**, P. Bothra, A. Kulkarni, J.K. Norskov, S. Siahrostami

10:20 CATL 482. Calculations on water oxidation catalysis modify the expected mechanism from experiments. **A. Poater**, M. Solà, J. Luque-Urrutia

10:40 CATL 483. Doping carbon catalysis for oxygen reduction reaction. M. Liu, T. Fan, **Y. Liu**, Y. Min

11:00 CATL 484. Unconventional binary ZnO/ZrO₂ heterogeneous catalysts for direct dehydrogenation of isobutane to isobutene. **Y. Liu**, **M. Ke**

11:20 CATL 485. Direct 3D printing of catalytically active structures. **J. Manzano**, Z.B. Weinstein, A.D. Sadow, I.I. Slowing

11:40 CATL 486. Hydrogen-assisted synthesis of CeO₂-Al₂O₃ with enhanced oxygen vacancy density. **B. Chen**

Section E
Hampton Inn & Suites Convention Center
Fulton

Control of Zeolite Structure, Composition & Sites for Catalysis
Cosponsored by INOR
R. Gounder, W.F. Schneider, *Organizers*

S. Goel, *Organizer, Presiding*
D. Hibbits, *Presiding*

8:00 CATL 487. Materials based on halloysite nanotubes with structured mesoporous silica for sulfur reduction in fluid catalytic cracking. **A.P. Glotov**, N. Levshakov, B. Anikushin, A. Vutolkina, S. Lysenko, E. Ivanov, V. Vinokurov, Y.M. Lvov

8:20 CATL 488. Self-assembly of ZSM-5/SBA-16 with different morphologies and its hydrodesulfurization of dibenzothiophene and 4,6-dimethyldibenzothiophene. X. Wang, Z. Zhao, P. Zheng, J. Fan, **A. Duan**, C. Xu

8:40 CATL 489. Synthesis of mesoporous zeolites using nanocellulose as an inexpensive hard template. **T. Pilyugina**, S.L. Kobaslija, J. O'Brien, B.S. Hanna, S.C. Hayden, S. Fernandez

9:00 CATL 490. Control over the mesoporosity of zeolites for the improved accessibility to their acid sites. N. Linares, E. De Oliveira Jardim, E. Serrano, **J. Garcia Martinez**

9:20 Intermission.

9:40 CATL 491. Synthesis protocols for the encapsulation of active and stable Au, AuPt, and AuPd nanoparticles within the protected void environment of zeotypes. **T. Otto**, S.I. Zones, E. Iglesia

10:00 CATL 492. Synthesis and characterization of tin, tin/aluminum, and tin/boron containing MFI zeolites. **M. Shahami**, R. Ransom, D.F. Shantz

10:20 CATL 493. Consequences of zeolitic vs. amorphous supports on the catalytic activity and stability of Ti(IV) and Fe(III) centers. **N. Grosso Giordano**, A.J. Yeh, M. Aigner, C. Schroeder, A. Solovyov, A. Okrut, N. Marinković, H. Koller, S.I. Zones, A.S. Katz

10:40 CATL 494. Synthesis and growth kinetics of zeolite SSZ-39. **R. Ransom**, J. Coote, R. Moulton, F. Gao, D.F. Shantz

Section F
Hampton Inn & Suites Convention Center
Cottonmill

General Catalysis

A. Savara, *Organizer*
S. Kattel, *Presiding*

8:00 CATL 495. CO₂ hydrogenation to CH₃OH on Cu/oxide catalysts. **S. Kattel**, J.G. Chen, P. Liu

8:20 CATL 496. Design of ionic polymer catalysts for the synthesis of cyclic carbonates from CO₂ and epoxides. **F.D. Bobbink**, P. Dyson

8:40 CATL 497. Hierarchically porous monoliths for fixed bed catalysis. **M.G. Bakker**

9:00 CATL 498. Catalytic performance of different zeolite catalysts for oligomerization of 1-butene. **Z. Lei**, M. Ke

9:20 CATL 499. Feasible synthesis of hydroxyapatite-supported palladium nanoparticles with controllable size and distribution and their enhanced catalytic activity. **X. Zhang**

9:40 CATL 500. Deep hydrodesulfurization over nickel phosphide on modified alumina supports. **M.E.**

[†]Cooperative Cosponsorship