



DECHEMA

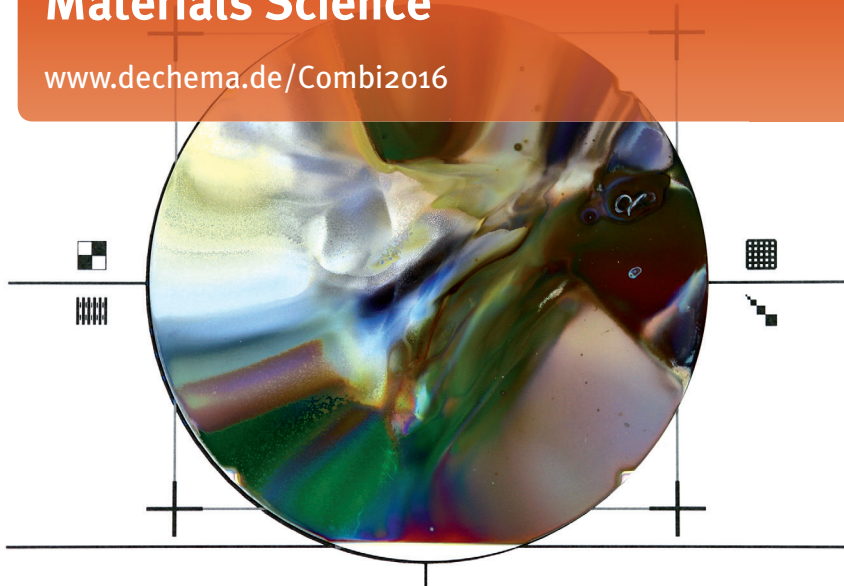
Gesellschaft für Chemische Technik
und Biotechnologie e.V.

PROGRAMME

26 – 28 September 2016
University Jena, Germany

9th International Conference on Combinatorial and High-Throughput Materials Science

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SUPPORTED BY:



seit 1558

Friedrich-Schiller-Universität Jena

Monday, 26 September 2016

Room: HS ZAF

08:30 **Registration**09:00 **Conference Opening**

SESSION 1: POLYMERS AND BIOMATERIALS

Chair: E. Amis; The University of Akron/USA

09:05 **KEYNOTE 1**
Science in the valley of death
 E. Amis¹; ¹ The University of Akron/USA

09:45 **KEYNOTE 2**
High throughput approaches for developing amphiphile self-assembly materials
 C. Drummond¹; ¹ RMIT University, Melbourne/AUS

10:25 **Combinatorial laser-assisted microarray technology for the synthesis of chemical compounds**
 T. Foertsch¹; D. Mattes¹; A. Nesterov-Mueller¹; F. Breitling¹; F. Loeffler¹; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D

10:50 **Coffee Break**

SESSION 2: POLYMERS AND BIOMATERIALS

Chair: U. Schubert; Friedrich-Schiller-University Jena/D

11:20 **KEYNOTE 3**
High-Throughput Polymer Materials Science for Directed Assembly of Polymer Thin Films
 A. Karim¹; ¹ The University of Akron/USA

12:00 **Polymerization of ethylene oxide under controlled monomer addition via a mass flow controller for tailor made polyethylene oxides**
 J. Vitz¹; T. Majdanski¹; A. Meier¹; P. Lutz²; U. Schubert¹; ¹ Friedrich-Schiller-University Jena/D; ² Institut Charles Sadron, University of Strasbourg/F

12:25 **High-throughput sequence-controlled polymerizations for the synthesis of novel gradient copolymers**
 C. Guerrero-Sanchez¹; S. Harrison²; J. Ulbrich³; I. Alvarez-Moises³; G. Festag³; U. Schubert⁴;
¹ Friedrich-Schiller-University Jena/D; ² Laboratoire des IMRCP, Université de Toulouse/F;
³ Laboratory of Organic and Macromolecular Chemistry, Friedrich Schiller University Jena/D;
⁴ Laboratory of Organic and Macromolecular Chemistry and Jena Center for Soft Matter, Friedrich Schiller University Jena/D

12:50 **Lunch Break**

Monday, 26 September 2016

Room: HS ZAF

SESSION 3: POLYMERS AND BIOMATERIALS

Chair: D. Brinz; Robert Bosch GmbH, Waiblingen/D

- 14:05 **KEYNOTE 4**
Concepts and Strategies in Automating Life Science Laboratories – What`s next?
K. Thurow¹; ¹ celisca/D
- 14:45 **High-throughput formulation of nanoparticles for structure-property investigations**
S. Schubert¹; A. Vollrath¹; I. Perevyazko¹; U. Schubert¹; ¹ Friedrich-Schiller-University Jena/D
- 15:10 **Advances in polymer screening for gene delivery approaches**
A. Träger¹; A. Vollrath¹; S. Schubert¹; U. Schubert¹; ¹ Friedrich-Schiller-Universität Jena/D
- 15:35 **Coffee Break**

SESSION 4: COATINGS, RESINS & SURFACES

Chair: J. Paul; Flamac, a division of SIM vzw, Zwijnaarde/B

- 16:05 **Combined High-throughput and Machine Learning Technique to Develop Multi-Principal Component Alloy Coatings**
B. Ruiz-Yi¹; J. Hu¹; J. Bunn¹; J. Hattract-Simpers¹; ¹ University of South Carolina, Columbia/USA
- 16:30 **High throughput analysis of alloy oxidaiotn and passivation**
M. Payne¹; J. Miller¹; A. Gellman¹; ¹ Carnegie Mellon University, Pittsburgh/USA
- 16:55 **High Throughput screening to implement HLD-NAC surfactant selection**
S. van Loon¹; A. Gutierrez¹; J. Martinez Sanchez¹; ¹ VLCI, Amsterdam/NL
- 17:20 **Cheap and robust 3D printed applicators for use in robotic high-throughput film application**
P. van den Berg¹; ¹ Nuplex BV, Bergen op Zoom/NL

SESSION 5: CATALYSIS

Chair: J. Paul; Flamac, a division of SIM vzw, Zwijnaarde/B

- 17:45 **Unlock Your Materials Space**
J. Grace¹; ¹ Chemspeed Technologies AG, Augst/CH
- 20:00 **Conference Dinner at the “Botanical Garden”** (20:00 – 23:00)
Fürstengraben 26, 07743 Jena
sponsored by the **Evonik Technology & Infrastructure GmbH**
- 21:00 **Guided Tour through the “Botanical Garden”**

Tuesday, 27 September 2016

Room: HS ZAF

08:30 **Registration****SESSION 6: ELECTRONIC MATERIALS & SENSORS, ENERGY PRODUCTION AND STORAGE***Chair: K. Stöwe; TU Chemnitz/D*

08:30 **KEYNOTE 5**
Combinatorial Synthesis and High Throughput Screening of Solid State Materials and Composites in Devices

B. Hayden¹; ¹ University of Southampton/UK

09:10 **Compositionally induced bandgap tuning of niobium-based combinatorial anodic oxides**
 A. Mardare¹; P. Bleckenwegner¹; W. Limberger¹; C. Mardare¹; C. Cobet¹; A. Hassel¹;
¹ Johannes Kepler University Linz/A

09:35 **High throughput experimentation of CdSe quantum dot nanocrystals for reproducibility and process-structure-property relationships studies**
 A. Mahmoud¹; J. Walter²; P. Herre²; I. Levchuck³; C. Brabec³; W. Peukert²; D. Segets²;
¹ Lehrstuhl für Feststoff- und Grenzflächenverfahrenstechnik Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen/D; ² Institute of Particle Technology (LFG), Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen/D; ³ Materials for electronics and energy technology (i-MEET), Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen/D

10:00 **High throughput synthesis and multi-dimensional analysis of Perovskite films**
 D. Segets¹; A. Mahmoud¹; E. Reinhardt¹; M. Distaso¹; W. Peukert¹; ¹ Institute of Particle Technology (LFG), Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen/D

10:25 **Coffee Break****INTRODUCTIONS WORKSHOPS**

11:10 **WORKSHOP 1:**
 A) Business Case: HTE-Service Provider
 B) Interface Academia-Industry
 C) Building an academic career with HTE

11:40 **WORKSHOP 2:**
 A) Business Case: HTE-Service Provider
 B) Interface Academia-Industry
 C) Building an academic career with HTE

12:10 **Summary & Discussion Workshop**13:00 **Lunch Break**

Tuesday, 27 September 2016

Room: HS ZAF

SESSION 7: CATALYSIS

Chair: H. Zanthoff; Evonik Technology & Infrastructure GmbH, Marl/D

- 14:15 **KEYNOTE 6**
Using high-throughput approaches to unravel structure-property relationships for heterogeneous catalysts
 K. Mingle¹; E. Sasmaz¹; C. Wen¹; J. Hattrick-Simpers¹; J. Lauterbach¹; ¹ University of South Carolina, Columbia/USA
- 14:55 **Efficient Performance Testing of Commercial Catalysts for Hydroprocessing Applications**
J. Klein¹; J. Berg¹; A. Haas¹; F. Huber¹; M. Kirchmann¹; T. Sauer¹; ¹ hte GmbH, Heidelberg/D
- 15:20 **Optimization of catalyst composition for direct hydrogenation of CO₂ to fuels and lower olefines**
 U. Rodemerck¹; M. Holena¹; A. Barkschat¹; D. Linke¹; E. Wagner²; M. Baerns³; ¹ Leibniz-Institut für Katalyse an der Universität Rostock e.V., Rostock/D; ² G.I.A.N.T. AG, Zug/CH; ³ Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D
- 15:45 **Performance testing of hydro desulphurization catalysts**
R. Moonen¹; E. Ras¹; ¹ Avantium, Amsterdam/NL
- 16:10 **Coffee Break**

SESSION 8: CATALYSIS

Chair: J. Klein; hte GmbH, Heidelberg/D

- 16:40 **High-Throughput Screening approach to new catalysts for total oxidation of methane from gas fueled lean burn engines**
T. Lenk¹; A. Gärtner¹; R. Kiemel²; S. Casu²; C. Breuer²; K. Stöwe¹; ¹ TU Chemnitz/D; ² Heraeus Deutschland GmbH & Co KG, Hanau/D
- 17:05 **Quantum Chemical High-Throughput-Screening of Materials and Catalysts**
M. Chęcinski¹; K. Stier¹; ¹ CreativeQuantum GmbH, Berlin/D
- 17:30 **KEYNOTE 7**
HTE is more than just buying a robot...: Clariant launches a new high tech lab designed to strike a highly productive balance between mechanized research and High Throughput experimentation
L. Kemp¹; ¹ Clariant Produkte (Deutschland) GmbH/D
- 18:10 **POSTER PARTY with Fingerfood and Drinks** (18:10 – 20:00)
 sponsored by the **Robert Bosch GmbH**

Wednesday, 28 September 2016

Room: HS ZAF

08:00 **Registration**

SESSION 9: ELECTRONIC MATERIALS & SENSORS, ENERGY PRODUCTION AND STORAGE

Chair: A. Ludwig; Ruhr-Universität Bochum/D

08:30 **KEYNOTE 8**
The Materials Design Engine: Integrating computation, synthesis and measurement for high-throughput materials discovery
A. Cooper¹; ¹ University of Liverpool/UK

09:10 **KEYNOTE 9**
Challenges in Advancing Materials-by-Design Beyond Equilibrium Materials
J. Perkins¹; ¹ National Renewable Energy Laboratory, Golden/USA

09:50 **Facilitating the Development of a “Virtual” High-Throughput (Combinatorial) Laboratory**
M. Green¹; Z. Trautt¹; N. Nguyen¹; A. Kusne¹; ¹ NIST, Gaithersburg/USA

10:15 **From high-throughput synthesis of nanocrystals towards upscaling of novel functional materials**
J. Paul¹; G. Huyberegts¹; P. Castelein¹; J. Clarebout¹; ¹ Flamac, a division of SIM vzw, Zwijnaarde/B

10:40 **Coffee Break**

SESSION 10: ELECTRONIC MATERIALS & SENSORS, ENERGY PRODUCTION AND STORAGE

Chair: W. Schrof; BASF SE, Ludwigshafen/D

11:10 **KEYNOTE 10**
Rapid Assessment of Magnet Alloys: From Soft to Hard
R. Ott¹; ¹ Ames Laboratory (USDOE), Ames/USA

11:50 **Multi-element substitution effect in cathode exploration for lithium ion battery**
K. Fujimoto¹; A. Aimi¹; Y. Yamaguchi¹; ¹ Tokyo University of Science, Noda/J

12:15 **High-Throughput Experimental Methods for Energy Materials Development**
A. Ludwig¹; ¹ Ruhr-Universität Bochum/D

12:40 **Closing Remarks**

12:55 **Lunch Break**

13:30 **Registration “Satellite Event” (Summerschool HTT 2016)**

- P1 Kinetic investigations of cross-linking reactions in automated parallel synthesizers and high-throughput characterization platforms**
 J. Ulbrich¹; C. Guerrero-Sanchez¹; I. Alvarez-Moises¹; J. Vitz¹; G. Festag¹; U. Schubert¹;
¹ Laboratory of Organic and Macromolecular Chemistry and Jena Center for Soft Matter, Friedrich Schiller University Jena/D
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- P2 Self-assembled nanostructures of Poly(n-alkyl methacrylate)s: Systematic investigation in non polar media.**
 C. Guerrero-Sanchez¹; A. Estrada-Ramirez²; O. Perez-Camacho²; R. Peralta-Rodriguez²;
 U. Schubert¹; E. Diaz Barriga-Castro²; ¹ Laboratory of Organic and Macromolecular Chemistry and Jena Center for Soft Matter, Friedrich Schiller University Jena/D; ² Centro de Investigación en Química Aplicada, Saltillo, Coahuila/MEX
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- P3 High-throughput kinetic investigations of the copolymerization of 1-octene with glycidyl methacrylate: reactivity ratios and potential applications**
 M. Rosales-Guzman¹; E. Saldivar-Guerra²; O. Perez-Camacho²; C. Guerrero-Sanchez³;
 S. Harrisson⁴; U. Schubert³; ¹ Centro de Investigación en Química Aplicada, Saltillo, Coahuila/MEX/Laboratory of Organic and Macromolecular Chemistry and Jena Center for Soft Matter, Friedrich Schiller University Jena/D; ² Centro de Investigación en Química Aplicada, Saltillo, Coahuila/MEX; ³ Laboratory of Organic and Macromolecular Chemistry and Jena Center for Soft Matter, Friedrich Schiller University Jena/D; ⁴ Laboratoire des IMRCP, Université de Toulouse/F
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- P4 New insights on the LCST behavior of Poly[2-(dimethylamino)ethyl methacrylate] through systematic high-throughput investigations**
 R. Yañez-Macias¹; C. Guerrero-Sanchez²; I. Alvarez-Moises²; R. Guerrero-Santos¹; U. Schubert²;
¹ Centro de Investigación en Química Aplicada (CIQA), Saltillo/MEX; ² Laboratory of Organic and Macromolecular Chemistry (IOMC) and Jena Center for Soft Matter (JCSM), Friedrich Schiller University Jena/D
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- P5 Synthesis of peptoids via a combinatorial laser-assisted microarray technology**
 D. Mattes¹; ¹ KIT Karlsruhe, Eggenstein Leopoldshafen/D
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- P6 Designed Synthesis of Cobalt Oxide Total Oxidation Catalysts**
 K. Mingle¹; E. Sasmaz¹; C. Wen¹; J. Hattrick-Simpers¹; J. Lauterbach¹; ¹ University of South Carolina, Columbia/USA
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- P7 Catalyst libraries with discrete composition spreads: preparation via inkjet printing and characterization by micro-spectroscopy**
 P. Fleischer¹; M. Weber²; K. Stöwe¹; ¹ Technische Universität Chemnitz/D; ² Universität des Saarlandes/D
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- P8 High-Throughput Screening of new catalysts for Diesel soot oxidation including evaluation of different catalyst preparation methods and soot contact modes**
 S. Hebert¹; L. Hensgen²; K. Stöwe¹; ¹ Technische Universität Chemnitz/D; ² Universität des Saarlandes/D

- P9 **High-throughput approach for novel noble metal free catalysts for combined steam and carbon dioxide reforming of methane**
 M. Löttsch¹; E. Yi²; R. Lane²; K. Stöwe¹; ¹ TU Chemnitz, Chemnitz/D; ² University of Michigan, Ann Arbor/USA
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- P10 **High-Throughput Optimization of a New On-Substrate Sintering Process of Li₂CO₃ and CoO for High-Quality Epitaxial LiCoO₂ Thin Films on SrTiO₃ (001)**
 S. Maruyama¹; O. Kubokawa²; K. Naibu³; K. Fujimoto³; Y. Matsumoto¹; ¹ Tohoku University, Sendai/J; ² Tokyo Institute of Technology, Yokohama/J; ³ Tokyo University of Science, Noda/J
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- P11 **Establishment of spinel-type Li(Ni,Mn,Ti)₂O₄ reaction phase diagram and these electrode properties**
 M. Yoshimura¹; Y. Yamaguchi¹; A. Aimi¹; K. Fujimoto¹; ¹ Tokyo University of Science, Noda/J
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- P12 **Discovering Photocathode Materials and Hydrogen Evolution Catalysts by High-Throughput Experimentation**
 H. Stein¹; R. Gutkowski¹; C. Eberling¹; M. Scherbeck¹; W. Schuhmann¹; A. Ludwig¹;
¹ Ruhr-Universität Bochum/D
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- P13 **Electrode properties of layered-type Li(Ni,Co,Fe)_{0.85}Ti_{0.15}O₂**
 K. Nanbu¹; Y. Yamaguchi¹; A. Aimi¹; K. Fujimoto¹; ¹ Tokyo University of Science, Noda/J
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- P14 **Optical High-Throughput Screening of electro-catalysts based on mixed metal oxides and combinatorial search for new fuel cell electro-catalyst support materials including a comparison of different synthesis methods for titania based mixed metal oxides**
 D. Reichert¹; C. Dogan²; F. Welsch²; T. Schwarz¹; W. Maier²; K. Stöwe¹; ¹ Technische Universität Chemnitz/D; ² Saarland University, Saarbrücken/D
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- P15 **Combinatorial search and comparison of different synthesis methods for new fuel cell electrocatalyst support materials**
 A. Seifert¹; M. Weber²; K. Stöwe¹; ¹ Technische Universität Chemnitz/D; ² Universität des Saarlandes/D
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- P16 **Determining the Stabilization Mechanism for High Entropy Alloys**
 B. Ruiz-Yi¹; J. Bunn¹; D. Stasak²; A. Mehta³; M. Besser⁴; M. Kramer⁴; I. Takeuchi²;
 J. Hattract-Simpers¹; ¹ University of South Carolina, Columbia/USA; ² University of Maryland, College Park/USA; ³ Stanford Synchrotron Radiation Lightsource, Menlo Park/USA; ⁴ Ames Laboratory, Ames/USA

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