

2019 PhD Symposium

November 7th 2019, Konventum

Gl. Hellebækvej 70, 3000 Helsingør

Program

08:30	Registration and coffee with bread at Konventum (room: Damgaardssalen)
09:00	Welcome by Head of Department, Erling H. Stenby
09:15	Before we start, Christin Pohl, PhD ChemClub

Session 1	<i>[Chair: Mathias Thor Nielsen]</i>
09:20 - 09:40	Alexandre Paolo Voute "Detection and control of bimolecular reactions from preformed weakly bound clusters"
09:40 - 10:00	David Nielsen "Electron Paramagnetic Resonance Spectroscopy on Cu-Zeolite Catalyst for Reduction of NO _x "
10:00 - 10:20	Christin Pohl "Biophysical Formulation Studies on an Anti-Microbial Peptide - The Effect of Point Mutations"
10:20 - 10:40	Daniel Hansen "Probing water diffusion in medical adhesives: Time-resolved chemical imaging & impedance spectroscopy"
10:40 - 11:00	Coffee Break

Session 2	<i>[Chair: Christin Pohl]</i>
11:00 - 11:30	Sanna Lund Diemer Senior Scientist <i>Roche Pharma Research and Early Development Roche Innovation Center Copenhagen A/S</i> "Oligonucleotide Synthesis: theoretical aspects and applications"
11:30 - 11:50	Chengxin Li "Structural, biosynthetic and serological cross-reactive elucidation of capsular polysaccharides from <i>Streptococcus pneumoniae</i> "
11:50 - 12:10	Fatemeh Keshavarzi "Model sunscreen behavior on TEWL and sweat simulators"
12:10 - 13:10	Lunch

Session 3	<i>[Chair: Mike Steffen Bernhard Jørgensen]</i>
13:10 - 13:40	Pablo Beato Lead Scientist <i>Atomic-Scale Analysis Department in R&D, Haldor Topsøe A/S</i> “Direct conversion of methane to methanol – still a dream reaction?”
13:40 - 14:00	Jing Tang “Sulfite Oxidase Bioanodes for Sulfite/O ₂ Biofuel Cells Based on Functionalized Graphene”
14:00 - 14:20	Johannes Eiler “An <i>In Vitro</i> Model to Evaluate the Performance of Skin Adhesives during Perspiration”
14:20 - 14:40	Mingli Liang “Relaxed Goldschmidt tolerance causes the change of structures and properties in two-dimensional Ruddlesden-Popper perovskites”
14:40 - 15:40	Photo-shoot Poster session (no.1-22) (room B10)
Session 4	<i>[Chair: Alexandre Paolo Voute]</i>
15:40 - 16:00	Natalia Teresa Skawinska “Towards the structure of human tryptophan hydroxylase isoform 2”
16:00 - 16:20	Simone Vestermann Samuelsen “Development and Mechanistic Investigation of the Manganese(III) Salen-Catalyzed Dehydrogenation of Alcohols”
16:20 - 16:40	Tao Jiang “Modification of an Aminated Surface Based on Polyelectrolyte Multilayers”
16:40 - 17:00	Wei Huang “Microwave-Assisted Crystalline and Morphology Evolution of Flower-like Fe ₂ O ₃ /Fe Doped K-birnessite Composite and its Application for Lithium Storage”
17:00 - 17:30	Poster session (no. 23- 45) (Foyer)
17:30 - 18:00	Free discussion
Dinner	
18:30	Conference dinner Announcement of the winner of the poster prize Announcement of the winner of the best oral prize Announcement of the winner of most correct answers in the oral quiz

Thanks to our sponsors



Titles poster session

1. **Amalie Nørskov**
"A novel dual drug-candidate for treatment of obesity-related type 2 diabetes"
2. **Anders Øwre**
"Design, synthesis and characterization of Metal-Organic Frameworks (MOFs) in the pursuit of novel conductive and magnetic materials"
3. **Charlotte Nybro Dansholm**
"Exploiting phosphate recognition and templates to drive the dynamic enzymatic synthesis of oligosaccharides"
4. **Charlotte Uldahl Jansen**
"A Novel Site-Selective Bioconjugation Strategy for the Synthesis of Energy Harvesting Protein-Conjugates"
5. **Dmytro Mihrin**
"THz Cluster Spectroscopy in *Para*-Hydrogen: Design of a Cryogen-Free Synthesis Apparatus and the Application for Weakly Bound $(\text{OCS})_m \cdots (\text{H}_2\text{O})_n$ Cluster Molecules"
6. **Faliu Yang**
"General strategy for synthesizing porous organic polymer"
7. **Fangyuan Diao**
"Ni-Fe-P coated nickel phosphide rods on the nickel foam as a bi-functional electrocatalyst for overall water splitting"
8. **Fernando De Azevedo Medeiros**
"Calculation of geochemical reactions in CO₂ EOR/sequestration processes"
9. **Frederik Hegaard**
"Friction on the molecular scale"
10. **Giorgia Masciotta**
"Template enzyme synthesis of alpha-glucans"
11. **Huili Cao**
"Synthesis of Carbon Coated Zinc Vanadate Nanoparticles for Lithium-ion Batteries Application"
12. **Ida Marie Vedel**
"Characterization and stabilization of tryptophan hydroxylases"
13. **Jie Meng**
"Competitive roles of Dopant and Defect States on the Charge Carriers Dynamics in Mn Doped All Inorganic Halide Perovskite Quantum dots"
14. **Junjie Kang**
"On-site Surface Coordination Complexation via Mechanochemistry for Versatile Metal-phenolic Networks Films"
15. **Kai Gao**
"Hydrogenation of bio-derived compounds using Pd incorporated in zeolites"
16. **Katja Desiree Pedersen**
"Exploring functionalized graphene as alignment media in NMR"
17. **Katja Egeskov Grier**
"Advanced Bioconjugation Technologies: Antibody Drug Conjugates in Cancer Treatment"
18. **Klaus August Moltved**
"Accuracy and precision of computational methods for transition metal hydrides and oxides"

19. **Koosha Ehtiati**
"Synthesis and characterization of poly (ionic liquid) brushes with various hydrophilicity and monomer bulkiness"
20. **Kristoffer Hauberg Rasmussen**
"Encapsulation of metal particles in zeolites for selective catalysis"
21. **Laura Voigt**
"Low valent metal-organic frameworks"
22. **Luca Piccirilli**
"Homogeneous catalysis for low-temperature hydrogen production from alcohols"
23. **Lucas Dos Santos Mello**
"Unsymmetrical Iron(II) and ruthenium(II) PNP complexes as catalysts for methanol and ethanol dehydrogenation"
24. **Marta Lopez Vidal**
"Development of quantum chemical methods to study X-ray spectroscopies"
25. **Mathias Thor Nielsen**
"Can polynuclear metal clusters behave as "extended" organometallic complexes?"
26. **Mike Steffen Bernhard Jørgensen**
"Conversion of Ethyl Levulinate to γ -Valerolactone Using PNP-pincer Complexes"
27. **Mikkel Burggraaf Buendia**
"Novel polymerizable scaffold for Trost ligands: Highly efficient reusable Trost ligands for Asymmetric Allylic Alkylation"
28. **Mikkel Krell-Jørgensen**
"A modular electrochemical flow reactor for automated organic synthesis"
29. **Niklas Rosendal Bennedsen**
"Porous organic polymers in heterogeneous fine chemical catalysis: concept and results"
30. **Nikolaj Sten Troelsen**
"Synthesis of diverse and three-dimensional fluorinated fragments for fragment-based drug discovery"
31. **Ping Zhu**
"Catalytic glucose transformations over zeolites in acetone media"
32. **Qinying Pan**
"In-situ growth of organic-inorganic hybrid perovskite on covalent organic frameworks"
33. **Robert Andrew Biro**
"Climate effects on polyelectrolyte films and resulting ice adhesion"
34. **Rouzana Pulikkal Thumbayil**
"Selective Dehydrogenation of Bioethanol using Copper Supported on Mesoporous Carbon"
35. **Runtian Qie**
"Polydopamine Coatings with Controlled Surface Roughness Obtained via Multiple Step Deposition Method"
36. **Sakhitha Koranchalil**
"Selective Catalytic Hydrogenation of 5-HMF to Platform Chemical"
37. **Simone Louise Zacho**
"Encapsulation of Polyoxometalates in Porous Silica-based Shells"

38. **Suk Kyu Ko**
“Molecular understanding of the effects of stabilizing excipients during lyophilization of biopharmaceuticals”
39. **Thomas Edward Whitmarsh-Everiss**
“Synthesis of a sterol-derived compound library for phenotypic screening”
40. **Torsha Moitra**
“Inner shell photoabsorption and photoionization cross-sections using coupled cluster methods”
41. **Ulf Molich**
“BioXAS on Plastocyanin Reveals Effect of Photoreduction”
42. **Weiguang Jin**
“Enhanced Stabilization of RNA by water stable ferrous supramolecular cage”
43. **Xiaomei Yan**
“Enhanced direct electron transfer of fructose dehydrogenase immobilized on Au (111) single-crystal electrode”
44. **Yibo Yang**
“Molecular diffusion of reservoir fluid systems in porous media”
45. **Yulong Miao**
“Transition-Metal-Free Direct Alkylation of Amides with Alcohols Using Potassium tert-Butoxide”