

## **Invitation**

DTU Chemistry  
PhD School Symposium

*Dear Collaborators and Alumni*

*I am pleased to invite you to DTU Chemistry's Annual PhD School Symposium in collaboration with the PhD ChemClub. The symposium is a great opportunity for you to gain insight into the PhD students' scientific work from different research groups and to strengthen the relationship with DTU Chemistry. The program will include oral and poster presentations by PhD students and a lecture from an external speaker.*

*We look forward to see you.*

*Erling H. Stenby  
Head of Department, Professor*

**When:** 10 November 2016

**Where:** **Pharmakon Konferencenter**, Milnersvej 42, 3400 Hillerød

**Registration:** You must register before **24 October 2016** to Coordinator Maria Bundgaard, [mabu@kemi.dtu.dk](mailto:mabu@kemi.dtu.dk)

*Participation is free of charge. However, the registration is binding.*

## 2016 PhD Symposium

November 10<sup>th</sup> 2016, Pharmakon Conference Centre

### Program

8:30	Registration and coffee with bread at Pharmakon
9:00	Welcome by Head of Department, Erling H. Stenby
9:15	Before we start, Amalie Elise Modvig, PhD ChemClub
<b>Session 1</b>	Chair: <b>Peter Langelund Thomassen</b>
9:20 - 9:40	<b>Christos Tsanas</b> "Calculation of Simultaneous Chemical and Phase Equilibrium"
9:40 - 10:00	<b>Esben Folger Thomas</b> "Deracemization via Shaped-Pulse Dynamic Stark Control"
10:00-10:20	<b>Aurun Kumar Somavarapu</b> "Presenilin-1 a Membrane Protein: Understanding The Role of Structural and Chemical Properties in Alzheimer's Disease"
10:20-10:40	<b>Rouzana Pulikkal Thumbayil</b> "Selective Catalysis with Metal Nanoparticles in Porous Materials"
10:40-11:00	<b>Coffee Break</b>
<b>Session 2</b>	Chair: <b>Jorge Peiro</b>
11:00-11:40	<b>PhD Pharm Henrik Parshad</b> (Principal scientist at Zealand Pharma) "Physicochemical and Formulation Risk Assessment in the Discovery Phase for Parenteral Peptide Delivery"
11:40-12:00	<b>Gianluca Levi</b> "Direct Dynamics Studies of Transition Metal Complexes for Solar Energy Conversion"
12:00-12:20	<b>Peter Langelund Thomassen</b> "Atom-Efficient Strategy for NO <sub>x</sub> Removal Using Ionic Liquids"
12:20-13:20	<b>Lunch</b>

### Session 3

Chair: **Tine Maja Frederiksen**

13:20-13:40

**Arnab Halder**

“Bioengineered Graphene Based Flexible Biosensing Platform”

13:40-14:00

**Saeed Zajforoushan Moghaddam**

“Conformational Study of Thermo-Responsive Polymers in Salt Solutions”

14:00-14:20

**Nedjelko Seselj**

“Graphene-Supported Au@Pt Catalyst in Fuel Cells”

14:20-14:40

**Kim Thollund Mortensen**

“High-Throughput Screening Technology for Profiling of Substrates for Histone Deacetylase Enzymes: Rational Design of Selective HDAC Inhibitors”

14:40-15:20

**Coffee Break**

Photo-shoot and Coffee Break

### Session 4

Chair: **Amalie Elise Modvig**

15:20-15:40

**Christian Kjeldsen**

“DNP NMR of Enzymatic Carbohydrate Conversion”

15:40-16:00

**Jorge Peiro**

“Prodrugs Sensitive to Reactive Oxygen Species for the Treatment of Chronic Inflammatory Diseases and Cancer”

16:00-16:20

**Duncan Paterson**

“Flash for Thermal Reservoir Simulation”

### Poster Session

16:20-18:00

Poster session with drinks

16:20-16:50 Meet the author (odd numbered posters)

16:50-17:20 Meet the author (even numbered posters)

17:20-18:00 Free discussion

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

HALDOR TOPSØE 



For sponsoring the Symposium

## Titles poster session

1. **Amalie Elise Modvig**  
"Selective Oxidation of Glycolaldehyde to Glycolic Acid"
2. **Ana Rita Freitas Colaço**  
"Peptide Macrocycles as Inhibitors of class I HDACs"
3. **Andrea Mazziotta**  
"Ruthenium Catalyzed Dehydrogenative Decarbonylation of Primary Alcohols"
4. **Bo Jessen**  
"Development of Catalytic Reactions to Prepare Bio-Based Polymer Building Blocks"
5. **Carola Santilli**  
"The Manganese-Catalyzed Kumada Coupling Reaction"
6. **Daniel Bo Larsen**  
"Theoretical Studies of the Transition Metal Catalyzed Deoxydehydration Reactions"
7. **Diego Rolando Sandoval Lemus**  
"Flash Calculations Including Capillary Pressure and Adsorption"
8. **Emilie Nørmølle Underlin**  
"Synthesis of Arabinoxylan Fragments"
9. **Fabrizio Bottaro**  
"Metal-Catalyzed Acceptorless Alcohol Dehydrogenation"
10. **Fei Shen**  
"Laccase-3D Graphene as Catalysts for Oxygen Reduction Reaction in Biocathodes"
11. **Giuseppe Antonacci**  
"Manganese Catalyzed Cross Coupling Reactions"
12. **Gokce Engudar**  
"Development of Transmembrane Ammonium Sulfate and pH Gradient Liposomes for Combined PET/CT Imaging"
13. **Hajar Golshadi Ghalehshahi**  
"Hetero Coupling of Aryl Grignard Reagents with Oxygen as an Oxidant"
14. **Irene Tosi**  
"Zeolites Catalysts for the Hydrolysis of Glycosidic Bonds"
15. **Kasper Damgaard Tidemand**  
"The Regulatory Mechanism of the Active Site Loop in Tryptophan Hydroxylase 1"
16. **Line Abildgaard Ryberg**  
"Detemir-Albumin Interactions Studied by Small-Angle X-ray Scattering and in-silico Modelling"

17. **Mats Simmermacher**  
“Time-Resolved X-Ray Scattering of Electronic Wave Packets”
18. **Minwei Zhang**  
“Ultralight and Semi-Transparent Metal Oxide Papers Composed of Nanoporous Monolayers for Lightweight Energy and Sensing Applications”
19. **Mostafa Abedi**  
“Atomistic Mechanism of Extended Excited-state Lifetime of Fe(II) Polypyridine Complex Functionalized With Carboxyl Groups”
20. **Samuel Gilbert Elliot**  
“Tin-Catalysed Conversion of Carbohydrates to  $\alpha$ -hydroxy Esters”
21. **Tine Maja Frederiksen**  
“Receptor Binding Interactions and Solution Structure of Glucagon-Like Peptide-1 Analogues”
22. **Ulf Molich**  
“Improving Methods for XAS Studies of Metalloproteins”
23. **Vanessa Baj**  
“Development of Receptors for Aqueous Carbohydrate Recognition”
24. **Wenbo Wang**  
“Formulation of Organometallic Anticancer Compounds in Liposomes”
25. **Xianyi Cao**  
“Flexible and Free-Standing Supercapacitor Electrodes Based on Graphene/SnS<sub>2</sub> Nanosheet/Ag Nanowire Ternary Composite Papers”
26. **Alina Kulakova, Ritu Mann, Sowmya Indrakumar, Sujata Mahapatra and Andreas Tosstorf**  
“Protein-Excipient Interactions and Protein-Protein Interactions in Formulation”