

2020 PhD Symposium

January 28th 2021, DTU Chemistry

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Program

09:00	Welcome by Head of Department, Erling H. Stenby
09:15	Before we start, PhD ChemClub
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Session 1	<i>[Chair: Mikkel Krell-Jørgensen]</i>
09:20 - 09:40	Daniil Fedotov “Damped (linear) response theory within the resolution-of-identity coupled cluster singles and approximate doubles (RI-CC2) method”
09:45 - 10:05	Giorgia Masciotta “Template enzyme synthesis of alpha-glucans”
10:10 - 10:30	Huili Cao “Microwave-assisted fabrication of V ₃ O ₇ ·H ₂ O nanowires/reduced graphene oxide composite for aqueous zinc-ion battery application”
10:30 – 10:45	Coffee Break
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Session 2	<i>[Chair: Robert Biro]</i>
10:45 - 11:05	Fernando De Azevedo Medeiros “State Function-Based Flash Specifications for Open Systems: Application to Geochemistry”
11:10 - 11:30	Kai Gao “Mechanistic study of the conversion from ethanol to 1,3-butadiene over Zn encapsulated zeolite catalyst”
11:35 – 11:55	Katja Desiree Pedersen “Exploring graphene oxide as alignment media in NMR”
11:55 – 12:40	Lunch break

Session 3*[Chair: Sofie Slott]*

12:40 - 13:00

Qinying Pan

“Excited-State Dynamics in 2,2'-bipyridine-based 2D Covalent Organic Frameworks Bearing Metal Sites as Synergistic Photocatalysts”

13:05 - 13:25

Yulong Miao

“Chromium(III) Porphyrin-Catalyzed Dehydrogenation of Alcohols to form Imines”

13:30 - 13:50

Mathies Brinks Sørensen

“In-Situ NMR based Metabonomics of Microbial Secondary Metabolites”

13:50 – 14:05

Coffee break

Session 4*[Chair: Ida Marie Vedel]*

14:05 - 14:25

Xiaomei Yan

“Understanding the effects of self-assembled monolayers and metallic structure on direct electron transfer of fructose dehydrogenase on Au(111) and nanoporous gold electrodes”

14:30 - 14:50

Torsha Moitra

“Theoretical modelling of photoionization dynamical parameters”

14:50 - 15:00

Closing remarks (DTU ChemClub and Erling H. Stenby)

15:00 - 15:30

Coffee break

Free discussion

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