

NKS Quantum/Computational Chemistry annual meeting 2025

(Scroll to the end of this document for location information)

Monday October 20th

12:00 Lunch (MH-kantina)

13:00 Welcome

13:10 Roberto di Remigio Eikås (Algorithmiq):

Aurora: end-to-end quantum chemistry on quantum computers

14:00 Break (20 minutes)

Contributed session 1:

Chair: Per-Olof Åstrand

14:20 Federico Rossi

Convex Hartree-Fock theory: A simple framework for ground state conical intersections

14:40 Oliver Bohle

Hartree-Fock level density-potential inversion for periodic systems

15:00 Evgueni Dinvay

Multi-configurational optimization for two-electron systems

15:20 Vebjørn Hallberg Bakkestuen

Density-Functional Theory Exemplified by Application to Quantum Electrodynamical Models

15:40 Break with coffee (20 minutes)

Contributed session 2:

Chair: Luca Frediani

16:00 Marco Bortoli

Accurate Machine Learning Interatomic Potentials for Grignard Reagents

16:20 Lukas Baldauf

To inf-init and Beyond: Active Learning for Neural Network Potentials Meets Highly Parallelizable Path Sampling

16:40 Gautam Jha

Machine Learning Augmented Tight Binding Potentials

17:00 Break (10 minutes)

17:10 NKS chapter general assembly

18:10 Get to city center, check in to hotel

19:30 Conference dinner (HilDr)

Tuesday October 21st

Contributed session 3:

Chair: Bjørn-Olav Brandsdal

- 08:30** Sarangerel Quarcoo
Computational Insight into Catalyst Stability: Surprising Ligand Effects
- 08:50** Miguel Ángel Gaona Fernández
Computational Insights into the Kinetic Isotope Effect for H Activation in Platinum-Based Bimetallic Systems.
- 09:10** Mohamed Safy
Computational Design Rules for Amine-Assisted CO₂ Hydrogenation to Methanol: Mechanistic Investigation and Microkinetic Modeling
- 09:30** Break with coffee (20 minutes)

Contributed session 4:

Chair: Thomas Bondo Pedersen

- 09:50** Jan Haakon Melka
EOM-P-CCSD
- 10:10** Doroteja Lipovec
Implementing the Jacobian Transpose in CCSDT
- 10:30** Alice Balbi
The role of ionic contributions when computing dispersion interactions
- 10:50** Break (20 minutes)

Contributed session 5:

Chair: Michal Repisky

- 11:10** Ingrid Dybdal
Field-dependent Molecular Ionization Potentials by a Multipole Expansion of the Charge Distribution
- 11:30** Edvard Dyre Hansen
DFT predictions of ¹³C pNMR shifts of guest-loaded HKUST-1 MOFs based on Cu(II)-dimer models
- 11:50** Closing
- 12:00** Lunch (MH-kantina)
- 13:00** End

Conference dinner: Hildir Restaurant, Skippergata 11



Hildir Restaurant

4,5 ★★★★★ (422) · 1000 kr+

Restaurant · [X](#)

Oversikt

Meny

Anmeldelser

Om



Veibeskrivel
se



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Del

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📍 Skippergata 11, 9008 Tromsø

