# Program, NKS Quantum and Computational Chemistry 2019, Radisson Blu Royal Garden, Trondheim

## Tuesday October 8th

09.45-10.00 coffee/tea

10.00-10.50 general annual meeting for members

10.50-11.00 break

Chair: Astrid de Wijn
11.00-11.30 Ljiljana Pavlovic (UiT), Rhodium-catalyzed hydrocarboxylation with $CO_2$.
11.30-12.00 Johannes Kirchmair (UiB), Computational prediction of xenobiotic metabolism

12.00-13.00 lunch

Chair: Ole Swang
13.00-13.20 Einar Uggerud (UiO), Sonochemical hydroxylation of salicylic acid --- a mechanistic enigma
13.20-13.40 Marco Foscato (UiB), Changing oxidation state paradigms in ruthenium-catalyzed olefin metathesis
13.40-14.00 Julie Héron (UiO), Computational study on catalyst activation for the $Cu_2$AAC reaction
14.00-14.20 Diego García López (UiT), To bind or not to bind; mechanistic insights into metal-$CO_2$ interplays to consctruct C-C bonds

14.20-14.50 break

Chair: Titus van Erp
14.50-15.10 Sverre Løyland (UiO), Computational and experimental study of simple models for biological $CO_2$ fixation
15.10-15.30 Sander Roet (NTNU), Transition state based replica exchange interface sampling (TS-RETIS)
15.30-15.50 Fabian M. Faulstich (UiO), Numerical and theoretical aspects of the DMRG-TCC method exemplified by the nitrogen dimer

15.50-16.20 break

Chair: Per-Olof Åstrand
16.20-16.50 TBA
16.50-17.20 TBA
17.20-17.50 Trygve Helgaker (UiO)

18.00-19.30 poster session

20.00-- dinner

## Wednesday October 9th

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| Chair: | Einar Uggerud |
| 08.30-09.00 | Sigbjørn Løland Bore (UiO), Hybrid particle-field molecular dynamics under constant pressure |
| 09.00-09.20 | Stefan Andersson (Sintef), Evaporation and diffusion in inert and oxidizing systems |
| 09.20-09.50 | Titus van Erp (NTNU), What triggers dissociation of water? |
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| 09.50-10.20 | break |
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| Chair: | Thomas Bondo Pedersen |
| 10.20-10.50 | Lukas Konecny (UiT), Relativistic four-component linear damped response time-dependent density functional theory |
| 10.50-11.10 | Roberto Di Remigio (UiT), Diagrammatic coupled cluster Monte Carlo. |
| 11.10-11.40 | Sarai D. Folkestad (NTNU), Performance of multilevel CC2 and multilevel CCSD |
| 11.40-12.00 | Eirik F. Kjønstad (NTNU), Aspects of excited-state-dynamics using coupled cluster theory |
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| 12.00-13.00 | lunch |
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| Chair: | Luca Frediani |
| 13.00-13.20 | Bin Gao (UiT), General recurrence-relation generation scheme for molecular integral evaluation |
| 13.20-13.40 | Magnus Ringholm (UiT), Some software design lessons I have learned |
| 13.40-14.00 | Jógvan Magnus Olsen (UiT), Scalability of DFT-based QM/MM MD simulations using the MiMiC framework |
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| 14.00-14.30 | break |
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| Chair: | Johannes Kirchmair |
| 14.30-14.50 | Håkon Emil Kristiansen (UiO), Real-time time-dependent coupled-cluster for electron dynamics |
| 14.50-15.10 | Rolf Heilemann Myhre (NTNU), Core excitations in new CC3 implementation |
| 15.10-15.30 | Tor Strømsem Haugland (NTNU), Chemistry in QED cavities |
| 15.30-15.50 | André Laestadius (UiO), Guaranteed convergence of a regularized Kohn-Sham iteration in finite dimensions |
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| 15.50-15.55 | Concluding remarks |