

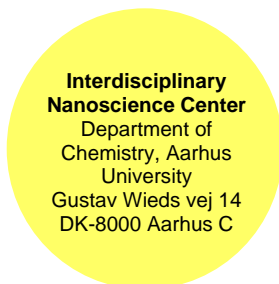
pNMR: The roots of the matter

Foundations and future challenges for theory and experiments of paramagnetic NMR

Schedule

Friday, July 8th

- 8.30 Registration
- 9.00 Michael Odelius (University of Stockholm)
[Welcome address](#)
- 9.15 **Willem van den heuvel** (University of Melbourne)
Theory of pNMR chemical shielding in open shell molecules
- 9.45 **Juha Vaara/Jiri Mares** (University of Oulu)
pNMR shieldings and couplings in the S.D.S realm
- 10.30 Coffee Break, *iNano Foyer*
- 11.00 **Alessandro Soncini** (University of Melbourne)
Theory of chiral discrimination in pNMR spectroscopy
- 11.30 **Martin Kaupp** (Technische Universität Berlin)
pNMR Computations from long-range PCSs in proteins to shifts in extended solids
- 12.00 Lunch, *Department of Chemistry*
- 13.30 **Frank Engelke** (Bruker BioSpin)
New Opportunities for Paramagnetic environments using Ultra-Fast MAS
- 14.00 **P.K Madhu** (TIFR, Mumbai/Hyderabad)
Overview of relaxation theory in paramagnetic systems
- 14.30 **Michael Odelius** (University of Stockholm)
Ab initio modeling of paramagnetic relaxation in metal complexes in solution
- 15.00 Coffee Break, *iNano Foyer*
- 15.30 **Björn Corzilius** (Goethe University)
Selective inversion of ¹³C resonances by DNP-driven and paramagnetically enhanced nuclear cross relaxation
- 16.00 **Anne Lesage** (CNRS Lyon)
Radicals for Efficient Solid-State Dynamic Nuclear Polarization
- 16.30 **Thomas Vosegaard** (University of Aarhus)
SIMPSON workshop
- 19.00 **Dinner**, *Department of Chemistry*



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Saturday, July 9th

- 9.00 **Phil Grandinetti** (Ohio State University)
2D NMR Measurements of Full Paramagnetic Shift Tensors of Quadrupolar Nuclei
- 9.30 **Brad Chmelka** (University of California Santa Barbara)
Paramagnetic NMR and scattering analyses of the structures, compositions, and properties of cerium-doped solid-state phosphors
- 10.00 **Elodie Salager** (CNRS Orléans)
In situ spectroscopic imaging of batteries containing paramagnetic materials
- 10.30 Coffee Break, *iNano Foyer*
- 11.00 **Andrew Pell** (University of Stockholm)
Measuring and interpreting paramagnetic shifts in materials science and biology
- 11.30 **Ulla Gro-Nielsen** (Syddansk Universitet)
Solid state NMR studies of paramagnetic, inorganic Ni(II) materials and complexes
- 12.00 Michael Odelius/Juha Vaara
[Concluding remarks](#)
- 12.00 Lunch, *Department of Chemistry*

Lunch will be served on Friday and Saturday, as well as Dinner on Friday, and will be free of charge for participants. However, please do attend if you said you would so.

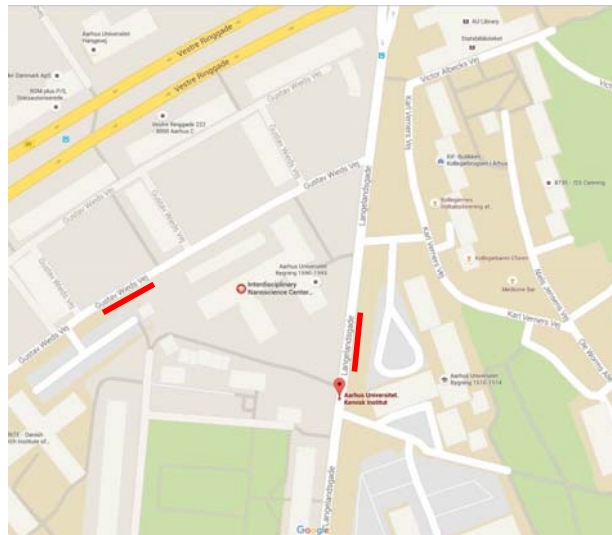
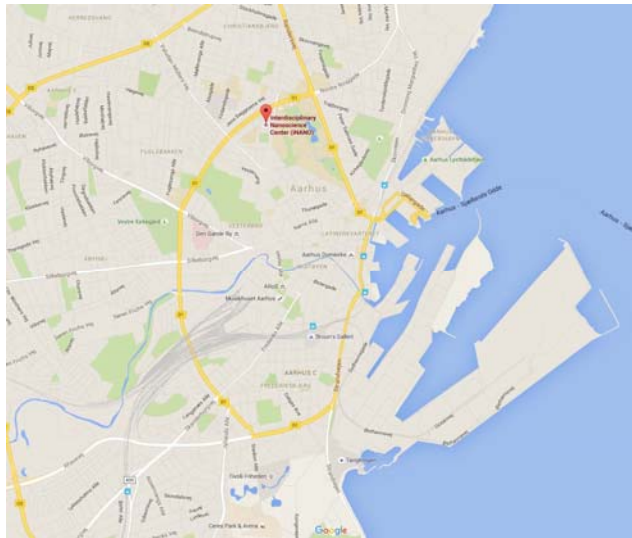
There will be no poster session.

The lecture theatre is located at basement level. When entering the building, cross the foyer, and go down the spiral staircase, following the "Auditorium" sign.

Wifi : To access Aarhus University wifi, please have a look at the following link
https://wifi.au.dk/guest_setup.php?lang=EN

Access Information

Maps and access information can be found on the iNANO website : <http://inano.au.dk/>, and more precisely here : <http://www.au.dk/en/about/organisation/find-au/buildingmap/?b=1592>



iNANO is located at the corner of Langelandsgade and Gustav Wieds Vej. The main entrance is from Gustav Wieds Vej where there is a parking lot with free parking spaces. An entrance is also available from Langelandsgade.



1- iNANO Building



2- Entrance Gustav Wieds Vej



3- Entrance Langelandsgade

iNANO is accessible by bus :

More information can be found on the [Midttrafik](http://www.midttrafik.dk) website.

You can also find a an online 'a - b' journey planner here : [Rejseplanen](http://www.rejseplanen.dk). It works for all Denmark.

The **Bus 16 towards Hasle** stops across the road (Langelandsgade) 100 meters from iNANO.

- Link to bus plan (<https://www.midttrafik.dk/koereplaner/bybusser/aarhus/bybusser-aarhus/16-hasle-park-all%C3%A9-holme-parkvej/koereplan?guid=606ac9db-e882-43db-a2ae-c19a1c0713ae>)

- Link to pdf with bus stops:
<https://www.midttrafik.dk/koereplaner/bybusser/aarhus/bybusser-aarhus/16-hasle-park-all%C3%A9-holme-parkvej/stoppesteder>



City buses in Aarhus:

The yellow city buses in Aarhus has self-service :

You enter the bus through any door, and buy your ticket at the ticket machine.

You must buy a ticket or stamp your multiride ticket (klippekort) immediately after entering the bus.

If you use mobile tickets, you must buy the ticket before entering the bus. If you have a bus pass or already have a valid ticket, you show this in case of a ticket inspection. If you don't have valid fare, you risk getting a penalty fare (750 kroner).

Travel Pass :

Offers unlimited travel in Aarhus (zone 301 – 313) on Midttrafik buses and Aarhus Nærbane (local rail line), including night buses. Aarhus Travel Pass is not valid for travel on other trains. Aarhus Travel Pass is available as a printout purchased through our website or as a mobile ticket in [Midttrafik app](http://www.midttrafik.dk)

Download [Midttrafik app](http://www.midttrafik.dk) in Google Play (Android) or App Store (iOS) or [buy and print Aarhus Travel Pass](http://www.midttrafik.dk).

Prices:

Duration:	adult/senior:
24 hours	80 kr.
48 hours	120 kr.
72 hours	160 kr.

Cash payment is usually the most expensive option per ride. It can however be a good option, if you only travel by bus a few times, while you're here.

The fares for bus rides (adult 16 years and older) are 20 DKK for zones 1-2.