DET 20. LANDSMØTE I KJEMI

29. - 30. oktober 2014, Norges Varemesse, Lillestrøm

Få faglig påfyll
og bli inspirert!

Industry Lecture

Guldberg-Waage foredrag

Analytisk kjemi

Kjemiens historie

Kjemiundervisning

Kvantekjemi og modellering

Matkjemi

Organisk kjemi og Makromolekylkjemi

Uorganisk kjemi og materialkjemi

Norsk Kjemisk Selskap

I samarbeid med Lab14

Velkommen til Det 20. Landsmøte i Kjemi

Norsk Kjemisk Selskap (NKS) inviterer alle med interesse for kjemi til Det 20. Landsmøte i Kjemi. Møtet arrangeres i nært samarbeid med LAB Norge og LAB14 på Norges Varemesse i Lillestrøm.

I 2014 er det 150 år siden Cato Maximilian Guldberg og Peter Waages oppdagelse av Massevirkningsloven. Dette vil markeres under landsmøtet ved at Norsk Kjemisk Selskaps høyeste utmerkelse, medaljen til minne om Guldberg og Waages massevirkningslov, deles ut til Professor Signe Kjelstrup fra NTNU for hennes innsats innen fysikalsk kjemi. Hun vil holde plenarforedraget første dag om sitt arbeid.

Industry Lecture presenterer et norsk industrieventyr. Geir Fonnum, Life Technologies, presenterer fremstilling og bruk av Ugelstadkuler inn mot diagnostikk, gensekvensering og cancer immunoterapi.

I løpet av messen vil Norsk Kjemisk Selskap ha en bemannet stand hvor vi vil informere om selskapet og de ulike oppgaver selskapet engasjerer seg i for å gjøre kjemi mer kjent for allmennheten. Stikk gjerne innom og bli "frelst"!

Det er laget et spennende og omfattende program for Landsmøtet. NKS har fått to nye faggrupper siden forrige møte og både Faggruppe for Kjemiundervisning og Faggruppe for Uorganisk Kjemi og Materialkjemi stiller med egne fagsesjoner. Årets landsmøte trekker flere deltagere enn noen gang tidligere.

Nytt denne gang er en pris til yngre forskere, initiert og finansiert av LAB Norge, i samarbeid med NKS, Norsk Biokjemisk Selskap (NBS) og Norsk Selskap for Medisinsk Biokjemi. Kandidater til prisen vil bli presentert etter plenarforedraget onsdag den 29. oktober, og prisen blir delt ut under "Happy Hour" senere på dagen.

Første dag av Landsmøtet avsluttes med en Landsmøtemiddag for de som har registrert seg til det – også den med rekordstor oppslutning i år!

Avslutningsvis vil vi benytte anledningen til å takke LAB Norge, Norges Varemesse og Teknolab AS for all støtte i form av velvillighet, entusiasme og økonomisk støtte, samt arrangementskomiteen for Landsmøtet 2014 for det arbeidet de har gjort for å sette sammen et spennende faglig program.

Vel møtt!

Øyvind Mikkelsen	**Harald Walderhaug**	**Nils Arne Jentof**
President	Generalsekretær	Leder av
NKS	NKS	Arrangementskomiteen

Innhold

Program

Abstracts

Organisasjonskomité

Nils Arne Jentoft	**Landsmøte-koordinator**
Harald Walderhaug	**Generalsekretær NKS**
Finn Knut Hansen	**Kasserer, webmaster og programhefte-redaktør**
Cathrine Thomsen	**Analytisk kjemi**
Bjørn Pedersen	**Kjemiens historie**
May Britt Stjerna	**Kjemiundervisning**
Heike Fliegl	**Kvantekjemi og modellering**
Grethe Modahl	**Makromolekyl- og kolloidkjemi**
Hans Blom	**Matkjemi**
Tore Bonge-Hansen	**Organisk kjemi**
Ragnhild Hanche	**Uorganisk kjemi og materialkjemi**

Sponsorer

Landsmøtet 2014 støttes av:

Norges Varemesse Lab14

LabNorge
Laboratorieleverandørene

Teknolab as
kromatografi spektroskopi yrkeshygiene

Vi skylder våre sponsorer stor takk for at dette arrangementet har blitt mulig.

Programplan og Fellesarrangement - 39. og 30. oktober

A1 (messe), rom 2

Onsdag 29.10

08.15 - 09.00	Registrering, kaffe/te
09.00 - 09.45	Åpning av Landsmøtet FE1 Guldberg Waage seremoni Ordstyrer: Øyvind Mikkelsen, President i Norsk Kjemisk Selskap
09.45 - 10.15	FE2 LAB Norges forskningspris
10.15 - 10.30	Kaffepause
10.30 - 12.00	Faggruppenes møter
12.00 - 14.00	Lunsjpause, besøk på messa
14.00 - ca 16.00	Faggruppenes møter
15.00 - 18.00	Happy hour
18.30 - ...	Landsmøtemiddag

Torsdag 30.10 **A1 (messe), rom 2**

08.15 - 09.00	Registrering, kaffe/te
Ordstyrer:	**Øyvind Mikkelsen**
09.00 - 09.45	**Industry Lecture:** FE3 Fremstilling og bruk av Ugelstadkuler inn mot diagnostikk, gensekvensering og cancer immunoterapi. *Geir Fonnum, Life Technologies AS, Svelleveien 29, 2004 Lillestrom*
09.45 - 10.00	Kaffepause
10.00 - 12.00	Faggruppenes møter
12.00 - 14.00	Lunsjpause, besøk på messa
14.00 -ca 16.00	Faggruppenes møter
ca 16.00	Slutt

Faggruppe for Analytisk kjemi

Norske Analysedager 2014

Rom Hordaland

Onsdag 29.10

08.15 - 09.00	Registrering, kaffe/te
09.00 - 10.15	Fellesarrangement
10.15 - 10.30	Kaffepause
	Dag 1: Kromatografi - Utfordringer og muligheter
Ordstyrer:	**Roland Kallenborn**
10.30 - 11.00	AN1 Beyond Chromatography: Real-time measurements of volatile organic compounds by PTR-MS. *Armin Wisthaler, Kjemisk institutt, Universitetet i Oslo.*
11.00 - 11.30	AN2 Nya GC-MS tekniker med potential att revolutionera miljöanalytisk kemi. *Peter Haglund, Kemiska institutionen, Umeå Universitet*
11.30 - 12.00	AN3 Barents Biocentre Lab – økt verdiskapning fra bioprospektering. *Terje Vasskog, Norut Tromsø (Northern Research Centre)*
12.00 - 14.00	Lunsjpause, besøk på messa
Ordstyrer:	**Catrine Thomsen**
14.00 - 14.30	AN4 Metabolomics – en ny "Canary of the coal mine" for medisinsk forskning. *Einar Jensen, Institutt for farmasi, Universitetet i Tromsø*
14.30 - 15.00	AN5 Oppdagelse og analyse av nye enzymaktiviteter. *Gustav Vaaje-Kolstad, Norges miljø- og biovitenskapelige universitet, NMBU*
15.00 - 15.30	AN6 Protein-adducts and DNA-adducts as sensitive biological parameters for both biological effect studies and environmental monitoring purposes *Daniela M. Pampanin, IRIS-International Research Institute of Stavanger*
15.30 - 16.00	AN7 Kartlegging av eksponering for Dieseleksos i Norsk arbeidsliv – hva er dieseleksos og hvordan kan vi måle dette? *Yngvar Thomassen, Statens arbeidsmiljøinstitutt (STAMI)*
16.00 - 18.00	Happy hour
18.30 - ...	Landsmøtemiddag

Torsdag 30.10

08.15 - 09.00	Registrering, kaffe/te
09.00 - 09.45	Fellesarrangement
09.45 - 10.00	Kaffepause
	Dag 2: Kvalitet i kjemiske analyser – Fra bestilling til rapportering av analyseresultat
Ordstyrer	**Elin Gjengedal**
10.00 - 10.05	Velkommen
10.05 - 10.50	AN8 Hvordan kan vi vite om sjømaten er trygg? Risikovurdering, biologisk variasjon og måleusikkerhet. *Amund Måge, Avdeling Trygg og sunn sjømat, Nasjonalt institutt for ernærings- og sjømatforskning (NIFES)*
10.50 - 11.25	AN9 Erfaringer og resultater fra 14 år med internasjonale ringtester for organiske miljøgifter i mat *Nanna Margrethe Bruun Bremnes, Folkehelseinstituttet*
11.25 - 12.00	AN10 Samlingsprov eller individuella prover för miljögiftsövervakning? *Sara Danielsson, Naturhistoriska riksmuseet, Stockholm*
12.00 - 14.00	Lunsjpause, besøk på messa
14.00 - 14.30	AN11 Assessing competence in the laboratory *Lorens P. Sibbesen, Training & Consultancy for laboratories, DK*
14.30 - 15.00	AN12 Analyse av fosfor i turbide vannprøver – Spesifikasjon av krav til analysemetode *Anne Falk Øgaard, Bioforsk, Ås*
15.00 - 15.30	AN13 Måleusikkerhet ved sum i multikomponentanalyser *Anders Torjuul Halvorsen, Laboratorium for klinisk biokjemi, Haukeland universitetssjukehus*
15.30 - 16.00	AN14 How to decide if a method is fit for intended use: The Fitness for Purpose of Analytical Methods: A Laboratory Guide to Method Validation and Related Topics *Lorens P. Sibbesen, Training & Consultancy for laboratories, DK*
16.00	Slutt

Faggruppe for Kjemiens historie

Kjemihistorisk årsmøte 2014

Rom Vestfold

Onsdag 29.10

08.30 - 09.00	Felles registrering
09.00 - 10.00	Plenarforedrag, fellesprogram
10.00 - 10.30	Kaffepause
Ordstyrer:	***Bjørn Pedersen***
10.30 - 11.15	HI1 Norsk krystallografi gjennom hundre år. *Carl Henrik Gørbitz, Universitetet i Oslo*
11.15 - 12.00	HI2 Rekonstruksjon av destillasjon på 1500-tallet *Fredrik Kirkemo, NTNU*
12.00 - 14.00	Lunsjpause. Besøk på messa
14.00 - 14.30	Årsmøte i faggruppen for Kjemiens historie
14.30 - 15.00	Kaffepause
15.00 - 15.30	HI3 Organisk kjemi i 1830 *Ragnar Bye, Farmasøytisk institutt, UiO*
15.30 - 16.00	HI4 Tidsskriftet Kjemis historie fra 1904 til i dag. *Bjørn Pedersen, Universitetet i Oslo*
16.00	Slutt

Faggruppe for Kjemiundervisning

Høstmøte 2014

Rom Rogaland

Onsdag 29.10

08.15 - 09.00	Felles registrering
09.00 - 09.45	Plenarforedrag, fellesprogram
10.15 - 10.30	Kaffepause
Ordstyrer:	***May Britt Stjerna***
10.30 - 11.00	Årsmøte i fagguppen
11.00 - 11.45	UN1 Kjemikalier og avfallshåndtering i skolen. *Brit Skaugrud, Skolelaboratoriet, Kjemisk institutt, Univ. i Oslo*
12.00 - 14.00	Lunsjpause. Besøk på messa
14.00 - 14.40	UN2 Organisk kjemi - hvordan få elever interessert i faget. *Yngve Stenstrøm, Institutt for kjemi, bioteknologi og matvitenskap, NMBU, Ås*
14.40 - 15.20	UN3 Kan hydrogen bære energi? *Per Odd Eggen, Skolelaboratoriet, NTNU, Trondheim*
15.20 - 16.00	UN4 Nanopartikler *Ola Nilsen, Kjemisk institutt, Univ. i OSlo*
16.00	Avslutning

Faggruppe for Kvantekjemi og modellering

Rom Romerike

Onsdag 29.10

08.15 - 09.00	Registrering, kaffe/te
09.00 - 09.45	Fellesarrangement
10.15 - 10.30	Kaffepause
	Sesjon 1:
Ordstyrer:	**Trygve Helgaker**
10.40 - 11.20	KM1 Orbital transformations for the localization of non-orthogonal molecular orbitals. *Ida-Marie Høyvik (NTNU)*
11.20 - 11.40	KM2 Redox processes of different transition metal triphenyl corroles and their impact on corrole aromaticity *Hugo Vazquez Lima (UiT)*
11.40 - 12.00	KM3 Local electric fields and ionization potentials in dielectric liquids. *Nazanin Davari (NTNU)*
12.00 - 14.00	Lunsjpause, besøk på messa
	Sesjon 2: Magnetic properties and method development
Ordstyrer:	**Einar Uggerud (UiO)**
14.00 - 14.20	KM4 Molecules in strong magnetic fields. *Erik Tellgren (UiO)*
14.20 - 14.40	KM5 Coupled-cluster theory for molecules in strong magnetic fields. *Stella Stopkowicz (UiO)*
14.40 - 15.00	KM6 Modeling of the adiabatic connection under the influence of external magnetic fields. *Sarah Reimann (UiO)*
15.00 - 15.20	KM7 High order geometric derivatives in quantum chemistry calculations: challenge, solution and implementation. *Bin Gao (UiT)*
15.20 - 15.40	KM8 A new approach to the calculation of vibrational wave functions *Clemens Woywod (UiT)*
15.40 - 16.00	Kaffepause

	Sesjon 3: Reactivity and catalysis
Orstyrer:	**Vidar Remi Jensen (UiB)**
16.00 - 16.20	KM9 Theory-Assisted Discovery and Development of Z-Selective Olefin Metathesis Catalysts. *Giovanni Occhipinti (UiB)*
16.20 - 16.40	KM10 Asymmetric transition-metal catalyzed hydrogenation reactions: Insights into the selectivity-determining factors. *Kathrin Hopmann (UiT)*
16.40 - 17.00	KM11 DFT Adventures on Structure, Reactivity, Development and New Concepts. *David Balcells (UiO)*
17.00 - 17.20	KM12 Nucleophilic substitution reactions of partially hydrated superoxide anions with alkyl halides. *Andrea Debranova (UiO)*
17.20 - 17.40	KM13 Doing Computational Chemistry faster and bigger. *Espen Tangen (Notur)*
17.40 - 18.30	Happy hour
18.30 - ...	Landsmøtemiddag
Torsdag 30.10	
08.15 - 09.00	Registrering, kaffe/te
09.00 - 09.45	Fellesarrangement
09.45 - 10.00	Kaffepause
	Sesjon 4: Materials modelling
Orstyrer:	**Per-Olof Åstrand (NTNU)**
10.00 - 10.40	KM14 Calculating transport properties from first principles: thermoelectric materials as a playground. *Ole Martin Løvvik (SINTEF/UiO)*
10.40 - 11.10	KM15 Chemical structure from photoelectron spectroscopy. *Knut Børve (UiB)*
11.10 - 11.40	KM16 Computational determination of a mechanism for silicon island formation in SAPO materials. *Ole Swang (SINTEF)*
11.40 - 12.00	KM17 Defect properties of functional oxides from first principles. *Tor Svendsen Bjørheim (UiO)*
12.00 - 14.00	Lunsjpause, besøk på messa
13.30 - 14.00	Division annual meeting

	Sesjon 5: Molecular dynamics and QM/MM methods
Orstyrer:	**Bjørn Olav Brandsdal (UiT)**
14.00 - 14.30	KM18 Modulation of protein function by micro-solvation effects: the puzzling case of cis-retinal binding in CRALBP. *Michele Cascella (UiO)*
14.30 - 15.00	KM19 Reaction path sampling using rare event simulation techniques *Titus van Erp (NTNU)*
15.00 - 15.20	KM20 Accurate QM/MM made cheaper: a hybrid approach to calculate polarizable embedding potentials. *Maarten Beerepoot (UiT)*
15.20 - 15.40	KM21 Thermal conductivity of carbon dioxide from non-equilibrium molecular dynamics: a systematic study of several common force fields *Thuat T. Trinh (NTNU)*
15.40 - 16.00	Kaffepause
	Sesjon 6: Method development
Orstyrer:	**Simen Reine (UiO)**
16.00 - 16.30	KM22 Divide wisely and conquer accurately: a strategy to please chemists who are notorioulsy demanding customers. *Luca Frediani (UiT)*
16.30 - 17.00	KM23 Molecular properties in the random phase approximation. *Thomas Bondo Pedersen (UiO)*
17.00 - 17.20	KM24 Cusp based DFT functionals. *Espen Sagvolden (SINTEF/UiO)*
17.20 - 17:40	KM25 Optimisation problems from exact DFT. *Ulf Ekström (UiO)*
18.00	Slutt

Faggruppe for Matkjemi

Tema: Matens kjemi i stadig endring – klarer vi å kontrollere den?

Vi ønsker å belyse ulike mat-perspektiver i et globalt, europeisk og nasjonalt lys, med fokus på matsikkerhet/trygghet og matkjemi i bred forstand.

Rom Nordland

Onsdag 29.10

08.15 - 09.00	Registrering, kaffe/te
09.00 - 09.45	Fellesarrangement
10.15 - 10.30	Kaffepause
10.30 - 12.00	Fri - finn på noe
12.00 - 14.00	Lunsjpause, besøk på messa
14.00 - 15.00	MA1 GMO i maten vår – et glimt inn i fremtiden *Askild Holck, Nofima AS*
15.00 - 16.00	MA2 Risikovurdering av GMO-produkter *Audun H. Nerland, Universitetet i Bergen*
16.00 - 16.30	MA3 Tradisjonell avl for bedre geitmelkskvalitet *Knut Erik Grindaker, Tine FoU*
16.30 - 17.00	MA4 Dyrking av grønnsaker i forskjellig klima-hva betyr det for innholdsstoffene? *Gunnar Bengtsson, Nofima AS*
17.00 - 18.00	Happy hour
18.30 - ...	Landsmøtemiddag

Faggruppe for Organisk kjemi og Makromolekyl og kolloidkjemi

Faggruppene har i år gått sammen om et felles program om organiske/myke materialer.
Vi lover 5 spennende foredrag om innovative organiske materialer!

Rom Akershus

Onsdag 29.10

08.15 - 09.00	Registrering, kaffe/te
09.00 - 09.45	Fellesarrangement
10.15 - 10.30	Kaffepause
Ordstyrer:	**Anne Fiksdahl**
10.30 - 11.15	OM1 DNA-Programmed Assembly of Molecules and Materials. *Professor Kurt Gothelf, Århus Universitet*
11.15 - 12.00	OM2 A tissue-like multifunctional 3D scaffold - Design and functionalization of resorbable matrices to adapt cell-material interactions. *Professor Anna Wistrand, KTH, Stockholm*
12.00 - 14.00	Lunsjpause, besøk på messa
Ordstyrer:	**Morten Brændvang**
14.00 - 14.45	OM3 Advanced Technical Textiles. *Dr. Klaus Opwis, Deutsches Textilforschungszentrum Nord-West gGmbH, Krefeld*
14.45 - 15.00	Kaffepause
Ordstyrer:	**Annette Bayer**
15.00 - 15.45	OM4 Triangulenium Salts. Synthesis, optical properties and self-assembly of cationic π-systems. *Professor Bo Laursen, Universitetet i København*
15.45 - 16.30	OM5 Endogenous-Inspired Hydrophobic Drug Delivery to Cancers: LDL-like Nano Particles Designed to "Put the Drug in the Cancer's Food". *Professor David Needham, Universitetet i Odense*
16.30 - 18.00	Happy hour
18.30 - ...	Landsmøtemiddag

Faggruppe for Uorganisk kjemi og materialkjemi

Rom Oslo

Onsdag 29.10	
08.15 - 09.00	Registrering, kaffe/te
09.00 - 10.15	Fellesarrangement
10.15 - 10.30	Kaffepause
	Sesjon 1
Ordstyrer:	**Anna Evans**
10.35 - 10.45	Velkommen *Truls Norby, UiO*
10.45 - 11.10	UM1 - KEYNOTE - Coatings for Anti-icing applications *Hilde Lea Lein (NTNU)*
11.10 - 11.25	UM2 Hyper-expanded FeSe-based superconductors *Kirill Yusenko (UiO)*
11.25 - 11.40	UM3 Development of novel biodegradable hybrid nanoparticles for cancer diagnosis and therapy. *Fuad Karimov (SINTEF)*
11.40 - 12.00	UM4 Engineering the morphology, composition and structure of PtRh Nanoparticles by Microwave Irradiation Synthesis *Maria Kalyva (UiO)*
12.00 - 14.00	Lunsjpause, besøk på messa
	Sesjon 2
Odstyrer	**Tor Svendsen Bjørheim**
14.00 - 14.25	UM5 - KEYNOTE - A master model for proton conducting materials *Truls Norby (UiO)*
14.25 - 14.40	UM6 Defect chemistry of hexagonal manganites from first principles *Sandra Helen Skjærvø (NTNU)*
14.40 - 14.55	UM7 Hydration and intercalation in Ruddlesden-Popper phases *Vegard Øygarden (UiO)*
14.55 - 15.10	UM8 Revisiting rhombohedral lead metaniobate: Crystal structure and functional properties *Gerhard H. Olsen (NTNU)*
15.10 - 15.25	UM9 Crystal chemistry and thermal properties of rare earth borohydrides *Christoph Frommen (IFE)*

15.25 - 15.40	UM10 Structural and magnetic aspects of $La_4(Co_{1-x}Ni_x)_3O_{10+\delta}$ *Marius Nagell (UiO)*
15.40 - 16.00	Kaffepause
16.00 - 17.00	Poster session
17.00 - 18.00	Happy hour
18.30 - ...	Landsmøtemiddag

Torsdag 30.10

08.15 - 09.00	Registrering, kaffe/te
09.00 - 09.45	Fellesarrangement
09.45 - 10.00	Kaffepause
	Sesjon 3
Odstyrer	**Nahum Maso Carcases**
10.05 - 10.30	UM11 - KEYNOTE - ZEG Power – more energy and less emissions *Bjørg Andresen (ZEG Power)*
10.30 - 10:45	UM12 Steam to hydrogen using high temperature proton ceramic electrolyser cells *Einar Vøllestad (UiO)*
10.45 - 11.00	UM13 Striking hydrogen uptake behavior differences in CPO-27 materials induced by metal substitution. *Mali Rosnes (UiB)*
11.00 - 11.15	UM14 Sodium- and potassium containing thin films by atomic layer deposition *Henrik H. Sønsteby (UiO)*
11.15 - 11.30	UM15 Luminecent lanthanide titanates by ALD *Per-Anders Hansen (UiO)*
11.30 - 11.45	UM16 Ferroelastic hardening in ferroelectric $(1-x)Bi_{0.5}K_{0.5}TiO_3 – xBiFeO_3$ (x = 0.8, 0.9) *Espen Tjønneland Wefring (NTNU)*
12.00 - 14.00	Lunsjpause, besøk på messa
14.00 - 14.30	Årsmøte i Faggruppen for uorganisk kjemi og materialkjemi

Sesjon 4

Ordstyrer	**Shay Alexander Robinson**
14.30 - 14.55	UM17 - KEYNOTE - Stability of carbon conductive additives at high operating voltages in Li-ion cathodes *Ann Mari Svensson (NTNU)*
14.55 - 15.10	UM18 Investigation of the electrical conductivity in LiAlO2 thin films deposited by Atomic Layer Deposition *Yang Hu (UiO)*
15.10 - 15.25	UM19 Effects of sintering additives on $BaZr_{1-x}Y_xO_{3-\delta}$: Densification, stability, and conductivity *Marie-Laure Fontaine (SINTEF)*
15.25 - 15.40	UM20 Additives in magnesium borohydride: local structure and effect on reversibility *Olena Zavorotynska (IFE)*
15.40 - 15.55	UM21 Powder synthesis and processing from nano to millimeter scale *Paul Inge Dahl (SINTEF)*
15.55 - 16:00	Avslutning
16.00	Slutt

Postere

Disse faggruppene har postere:

PU - Uorganisk kjemi og materialkjemi

PK - Kvantekjemi og modellering

(For abstracs henvises til nettsidene).

KM – Faggruppe for Kvantekjemi og modellering

KM1 **First Principles Modeling of Solid Acid Catalysis Supported by Experiments: From Kinetics to a Reactivity Descriptor**
Rasmus Y. Brogaard (UiO)

KM2 **The π→π✳ excitation energy of azo compounds by a combined charge-transfer and point-dipole interaction model**
Shokouh Haghdani (NTNU)

KM3 **Relativistic four-component calculations of indirect nuclear spin-spin coupling using hybrid functionals**
Stanislav Komorovsky (UiT)

KM4 **Multi-level coupled cluster theory**
Kristin Marie Skjelbred (NTNU)

KM5 **Mesoscopic modeling of DNA denaturation rates**
Oda Dahlen (NTNU)

KM6 **Gluing potential energy surfaces with rare event simulations**
Anders Lervik

KM7 **Molecular excitation energies with a range-separated second-order dynamical Bethe-Salpeter kernel**
Elisa Rebolini

KM8 **Real-time solution of the time-dependent Dirac-Coulomb equation**
Márius Kádek

PU – Faggruppe for Uorganisk kjemi og materialkjemi

PU1 **A new approach for correcting transport numbers of native and foreign ions in molten carbonates**
Anna Evans (UiO)

PU2 **A first-principles study of epitaxial interfaces between graphene and GaAs**
Astrid Marthinsen (NTNU)

PU3 **Local and average structure of BiFeO3 solid solutions**
Bo Jiang (NTNU)

PU4 **Metal supported proton ceramic electrolyser cells (PCEC) for renewable hydrogen production**
Elena Stefan (UiO)

PU5 **In situ characterization of hydrothermal synthesis of piezoelectric oxides**
Susanne Linn Skjærvøe (UiO)

PU6 **Perovskite to post-perovskite transition in NaFeF3**
Fabian L.M. Bernal (UiO)

PU7 **The effect of hybrid nanoparticle additives on barrier and mechanical properties of polymer blends as self-healing materials**
Huaitian Bu (SINTEF)

PU8 **In operando structural investigation of Na+ intercalation into the Prussian blue analogue Na1.35Mn[Fe(CN)6]0.83 · z H2O**
Jonas Sottmann (UiO)

PU9 **Ceramic composites of mixed ionic-electronic conductors as hydrogen membranes**
Jonathan M. Polfus (SINTEF)

PU10 **Enhancing the O2 permeability of CaTi0.85Fe0.15O3**
Jonathan M. Polfus (SINTEF)

PU11 **Novel precursors for silicon containing materials**
Karina B. Klepper (UiO)

PU12 **Computational study of molybdenum trioxide as an intermediate band material**
Katherine Izani (NTNU)

PU13 **Surprising rapid intercalation pseudocapacitance effects in amorphous LiFePO4**
Knut Bjarne Gandrud (UiO)

PU14 **The structural reason for hydrogen capacity loss in Fe-containing bcc alloys – a PDF study**
Magnus H. Sørby (IFE)

PU15 **Self-heating of ion conducting membranes**
Marie-Laure Fontaine (SINTEF)

PU16 **A study of Pt-electrode interfaces on Nb doped TiO2 by cyclic voltammetry and impedance spectroscopy**
Marit Norderhaug (UiO)

PU17 **Nano-layered silicon from calcium disilicide by the use of ammonium chloride or hydrogen chloride for the utilization as anode in lithium-ion-batteries**
Matthias Herrmann (UiO)

PU18 **Luminescent properties of europium titanium phosphate thin films deposited by atomic layer deposition**
Michael Getz (UiO)

PU19 **Electrical Properties of nonstoichiometric $Ba_{1+X}Zr_{0.85}Y_{0.15}O_{2.925}$ ceramics prepared by solid state reactive sintering**
Nahum Masó (UiO)

PU20 **Electrical properties of undoped and acceptor-doped $(LaO)_2SO_4$ ceramics**
Nahum Masó (UiO)

PU21 **Crystallisation and electrochemical investigation of α- and β-MoO_3 thin films deposited by Atomic Layer Deposition (ALD)**
Øystein S. Fjellvåg, Amund Ruud (UiO)

PU22 **First-principles study of structural stability, dynamical and mechanical properties of $Li_2FeSiPO_4$ polymorphs**
Ponniah Vajeeston (UiO)

PU23 **Investigation of Li+ insertion in columbite structured FeNb2O6 and rutile structured CrNb2O6 materials**
Pushpaka Samarasingha (UiO)

PU24 **Characterization of electrodes on ionic conductors with transport of more than one type of charge carriers**
Ragnar Strandbakke (UiO)

PU25 **Correlation between bulk and surface kinetics of proton conducting oxides**
Ragnhild Hancke (UiO)

PU26 **Development of high-performance ceramic sorbent for high-temperature CO2 separation and hydrogen production**
Saima Sultana Kazi (IFE)

PU27 **Hydrogen permeation and transport properties of BZY and GCO composites**
Sarmad W. Saeed (UiO)

PU28 **Impedance study of model electrodes for use in carbon containing atmospheres**
Shay Robinson (UiO)

PU29 **Modelling of surface conduction of porous oxides**
Sindre Stub (UiO)

PU30 **Dual-phase membrane for high temperature CO2 separation**
Wen Xing (SINTEF)

PU31 **Disordered crystal structure of MoO3 nanobelts**
Wojciech A. Sławiński (UiO)

Abstracts

FE - Fellesarrangement

FE1

Beregning av likevekt og transport med de små systemers metode (SSM)

Signe Kjelstrup

Institutt for kjemi, Norges Teknisk-Naturvitenskapelige Universitet

Foredraget tar for seg en ny metode til beregning av termodynamiske data[1-6]. Metoden er sentral for kjemikere og kalles de små systemers metode (SSM). To velkjente problemstillinger blir presentert for å illustrere metoden i bruk, adsorpsjon av CO2 på grafitt[6] og dissosiasjon av hydrogen i en temperaturgradient[5].

Ved likevekt mellom gas og adsorbert lag, eller i den kjemiske reaksjonen, viser jeg hvordan vi kan skaffe opplysninger om kjemisk potensial, aktivitetskoeffisienter, reaksjonsentalpier etc. fra en eneste simulering. Størrelsen på liten test-boks blir variert og variasjonen i partikkeltall i den lille boksen blir undersøkt, se Figur 1. Her ligger all informasjon om systemet ved gitte betingelser. SSM bygger på Hills metode for beregning av egenskaper til små system. Egenskapene til små og store system knyttes sammen med skaleringslover.

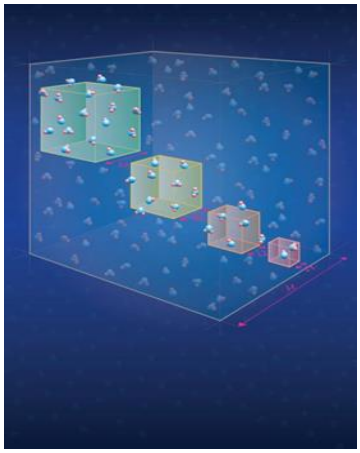

Fig.1. Små system av varierende størrelse i et reservoar som holder temperatur og konsentrasjon konstant.

Foredraget gir oversikt over diffusjonskonstanter som nylig er beregnet med metoden[2,4]. Beregningene stemmer svært godt overens med eksperimentelle resultater. Vi skal også se at transportegenskapene til en blanding påvirkes sterkt når komponentene deltar i en kjemisk reaksjon[5]. Irreversibel termodynamikk teori predikerer at en hittil ubrukt transportparameter, overført varme, forandrer blandingens varme- og masse overføringsegenskaper. Disse resultatene blir bekreftet ved simuleringer. Metoden[1-6] kan være nyttige for bedre modellering av katalyse, membrantransport eller adsorpsjonsprosesser.

Metoden SSM er til implementering i LAMMPS og vil bli åpent tilgjengelig i 2015.

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FE3

Fremstilling og bruk av Ugelstadkuler inn mot diagnostikk, gensekvensering og cancer immunoterapi.

Geir Fonnum

Life Techologies AS, Svelleveien 29, 2004 Lillestrøm, Tel (+47) 22061246

Geir Fonnum has M.Sc in Organic Chemistry from the Norwegian University of Science and Technology in 1985, and a PhD in the field of Organic/Polymer chemistry in 1989 at the same University. His industrial R&D career started in the Surface and interfacial group at Dyno Industries. In 1991 he started working with Ugelstad spheres for chromatography applications in first at Dynochrom and later at Pharmacia Biotech.

In 1999 he moved to Dyno Specialty Polymers which was acquired by Dynal in 2001. Dynal was acquired by Invitrogen in 2005, merged to Life Technologies in 2009 and was acquired by Thermo Fisher in 2014.

Geir has been leading the bead chemistry development at Dynal since 2001. During the last 15 years Dynal R&D has developed both magnetic and non-magnetic beads products for a broad range of applications ranging from *In vitro* diagnostics and proteomics to semiconductor DNA sequencing (Ion torrent) and beads for cancer immunotherapy. Dynal is at the moment the world leading supplier of magnetic beads for these applications.

In his talk Geir will show how Dynal uses the Ugelstad technology to produce magnetic beads for bioseparations. He will also show how Dynal uses different bead architectures to solve the requirements of different biological applications and also the results of the major cancer immunotherapy work.

AN - Analytisk kjemi

AN1

Beyond Chromatography: Real-time measurements of volatile organic compounds by PTR-MS

Armin Wisthaler

Kjemisk Institutt, Universitetet i Oslo

Chromatographic separation combined with mass spectrometric analysis (GC-MS, LC-MS) is usually used for speciation and quantification of volatile organic compounds (VOCs) in air. Chromatography is, however, time and labor intensive and off-line analysis does not give real-time analytical insights. I will herein demonstrate that, for a variety of analytes and matrices, direct sample introduction followed by chemical ionization mass spectrometric analysis, is a viable method for monitoring of VOCs in real-time.

Proton-Transfer-Reaction Mass Spectrometry (PTR-MS) (Fig. 1) combines the principles of
i) soft chemical ionization of VOCs (via protonation from H3O+ reagent ions), and
ii) linear and intrinsically quantitative analyte ion formation in an ion drift tube.

The method excels in high sensitivity (resulting in ppt level detection limits) and high measurement frequency (up to 10 Hz). Since its inception in the mid-1990ies, PTR-MS has become a leading technology in the on-line VOC analysis, spanning a number of research fields that include environmental chemistry (Fig. 2), food science, and life sciences. Selected application examples in these fields will be given.

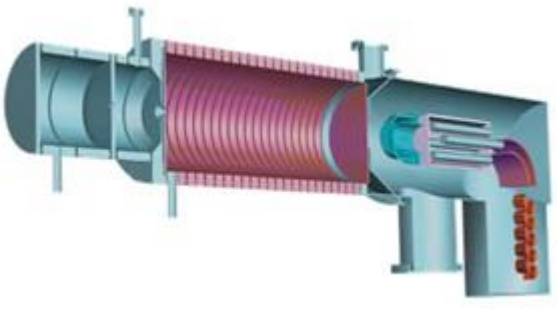

Fig. 1: Scheme of the PTR-MS instrument showing the glow discharge ion source (left), ion drift tube (center), and mass spectrometer (right)

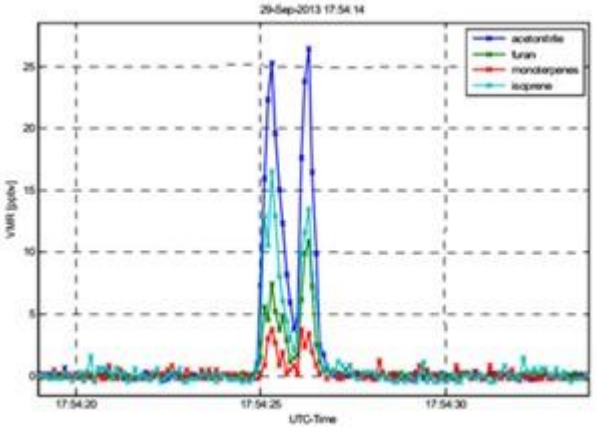

Fig. 2: 10-Hz VOC data obtained from a research airplane that sampled a forest fire plume (figure courtesy: M. Müller)

AN2

New gas chromatography-mass spectrometry (GC-MS) techniques that may revolutionize environmental analytical chemistry

Peter Haglund[1], Liz Humston-Fulmer[2], Ulrika Olofsson[1], Conny Danielsson[1]

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2 Leco Corporation, St. Joseph, MI 49085, USA.

In the modern society, large quantities of chemical substances are used, and more than 30 000 compounds are estimated to be in daily use in Europe, of which many will reach environment through e.g. the municipal sewage treatment plant (STP) effluents. In addition to that, natural production of biogenic halogenated compounds, e.g. marine toxins, may increase as a result of climate-induced change (CIC). Many of these chemicals are hazardous to humans and to the environment.

Often these anthropogenic compounds and marine toxins are present at trace levels together with much more abundant biogenic compounds. Thus, there is a need for tools to characterize, identify and quantify legacy and emerging contaminants present in this "chemical soup". Over the last decades, hyphenated techniques combining a chromate-graphic separation and mass spectrometry have proven to be well suited for such tasks. In this presentation we will focus on new and upcoming GC-MS techniques.

The separation power of conventional capillary GC is already quite good and it may be possible to accommodate several hundreds of peaks in a one-hour chromatogram. When combined with MS even more compounds can be resolved. By adding a second GC dimension with orthogonal selectivity the peak capacity will improve drastically. Using comprehensive two-dimensional GC (GCxGC) up to 10,000 compounds may be physically separated. When combined with rapid time-of-flight (TOF) MS and mass and spectral deconvolution algorithms it is possible to separate and characterize a significant share of GC amenable compounds present in complex environmental samples.

Identification may however still be a problem. If the sample constituents are not present in any of the large electron ionization (EI) MS libraries, or if there are several compounds with similar spectra, identification is not possible. In such cases GCxGC high-resolution TOF-MS can provide valuable complementary information on the element composition of molecular and fragment ions, which can be used in manual or in-silico structure elucidation.

In cases when EI do not produce molecular ions identification attempts are likely to fail and soft ionization techniques would be required. Traditional chemical ionization (CI) and atmospheric pressure CI often produce information of psedo-molecular ions, but it is sometimes difficult to know if this ion is protonated or not. Recently developed approaches for "soft-EI" may overcome this problem.

Currently, one of the biggest problem is to get sufficiently good software to efficiently process and quarry the data produced by the state-of-the-art hardware. Significant

improvements are needed in the peak picking, peak/spectral deconvolution and peak integration algorithms. It is also room for improvement in the tools for sample comparison and identification of compounds of interest. Both the functionality and degree of automation can be improved.

AN3

Barents Biocentre Lab - Økt verdiskapning fra bioprospektering

Terje Vasskog

Norut

Barents Biocentre Lab (BB Lab) er en bioinkubator i forskningsparken i Tromsø. Her kan både bedrifter, akademia og forskningsinstitutter få tilgang til laboratoriearealer og avansert instrumentering.

Det er en stor satsing på bioprospektering i Tromsø, både innenfor næringslivet og i ulike forskningsgrupper på UiT - Norges Arktiske Universitet. På BB Lab har de alle en mulighet til å benytte instrumentering de ikke ellers har tilgang til, møtes og diskutere idéer og utvikle samarbeidsprosjekter.

Per i dag har BB Lab samarbeid med en rekke sentrale aktører innen bioprospekteringen i Tromsø. MabCent (UiT) har lang erfaring innen den tradisjonelle marine bioprospekteringen. De samler inn organismer, ekstraherer, isolerer og bioaktivitetstester ulike forbindelser i stor skala. De isolerte forbindelsene gir ofte grunnlag for syntese av større mengder av de isolerte forbindelsene, eller analoger av disse for å videreutvikle forbindelsen. MabCent samarbeider per i dag med Norut på BB Lab om et prosjekt der slike syntetiserte forbindelser renses og karakteriseres før de skal testes for bioaktivitet.

Flere bedrifter er også etablert i BB Lab og jobber innenfor bioprospektering. Av de største er Barentzymes, et nyetablert selskap med 15 ansatte som jobber med enzymer fra organismer i arktiske farvann. Selskapet fokuserer på å utvikle nye enzymer til bruk innen industriell bioteknologi.

Også andre mindre bedrifter har etablert seg på BB Lab, og selv om hovedaktiviteten ikke er bioprospektering har flere av dem vært innom dette fagområdet gjennom samarbeid med ulike aktører. Et godt eksempel på dette er D'liver, et selskap som tilbyr spesialtilpassede forsøk for å bestemme leveropptak, distribusjon og metabolisme av ulike forbindelser. Kompetansen på dette området ble benyttet i et samarbeidsprosjekt med Marealis og Norut, der Marealis har oppdaget et marint peptid med bioaktivitet, og D'liver gjorde forsøk på mus med dette peptidet for å se på opptak og distribusjon, mens Norut analyserte peptidet i ulike prøver fra mus ved hjelp av LC-MS.

Andre aktører, som for eksempel Naturtjenester i Nord gjør også bioprospektering, men i Nord-Norske bær istedenfor marine organismer. I et samarbeidsprosjekt med Norut analyseres bærekstrakter for ulike forbindelser med gunstig helseeffekt.

AN4

Metabolomics – utfordringer og muligheter for kromatografi-MS

Einar Jensen

Institutt for farmasi, Universitetet i Tromsø

Metabolomics er en naturlig medspiller til både genomics og proteomics. Med å kombinere kunnskaper fra alle de ulike –omics kan nye pathogene patways oppdages. Metabolomics kan identifisere molekyler som kan brukes både som prognostikse og diagnostiske biomarkører og evt indikere at bruk av kostbare legemidler kan seponeres. Ulike deler av en typisk metabolomics workflow vil bli diskutert og hvor det vil bli lagt særlig vekt på hvilke muligheter og utfordringer ulike varianter av kromatografi-massespektrometri har innen metabolomics. Definisjon av metabolomics, study design og bioinformatikk vil og bli kort diskutert. Prosjektet ”ASIB – Advanced Studies of Inflammatory Bowel disease and related disorders” vil og bli presentert.

AN5

Oppdagelse og analyse av en ny enzymaktivitet

Gustav Vaaje-Kolstad

Norges miljø- og biovitenskapelige universitet

Mikroorganismer som anvender polysakkarider som næringskilde tar i bruk en rekke karbohydrataktive enzymer (CAZymes) for å oppnå en effektiv nedbrytningsprosess. For fire år siden oppdaget vi en ny enzymaktivitet som har vist seg å spille en viktig rolle i nedbrytningsprosessen, spesielt for solubilisering av uløselige polysakkarider som kitin og cellulose. Den nye enzymaktiviteten går under navnet «lytisk polysakkarid monooxygenase» (LPMO) og innebærer spalting av glykosidbindinger med en oksidativ mekanisme. LPMOene benytter et kopperatom til å aktivere molekylært oksygen, hvilket ved en ukjent mekanisme medvirker til oksidasjon av C1 eller C4 karbonet i glykosidbindingen. Dette gir brudd i polysakkaridkjeden og resulterer i dannelse av oligosakkarider med enten en aldonsyre (ved C1 oksidasjon) i reduserende ende eller en 4-ketoaldose (ved C4 oksidasjon) i ikke-reduserende ende. Det unike med LPMOene er at de utfører sin reaksjon direkte på overflaten av en polysakkaridkrystall. I foredraget vil jeg lede tilhørerne gjennom historien om hvordan en slik tilsynelatende åpenbar enzymaktivitet har forblitt uoppdaget i så mange år, samt hvordan vi løste de analytiske utfordringene relatert til separasjon og identifikasjon av de oksiderte oligosakkaridene.

AN6

Protein-adducts and DNA-adducts as sensitive biological parameters for both biological effect studies and environmental monitoring purposes

Daniela M. Pampanin

IRIS-International Research Institute of Stavanger

Petroleum related activities in Norway are conducted in shallow seas contiguous to the Norwegian coastlines and offshore in the North Sea. Monitoring and assessment of water quality is essential to survey the potential impact for these activities. Expanding oil exploitation to more vulnerable area, such as the Artic, requires the development of even more sensitive methods for the overall understanding of the impact of oil and chemical contamination in the sea. In the last 10 years, IRIS, in tight collaboration with Norwegian operators (Norsk olje & gass, previously known as OLF) and other national research institutions, has developed and performed monitoring of the impact of oil related activity in the North Sea.

Polycyclic aromatic hydrocarbons (PAHs) are common substituents found in crude oil. Since the occurrence and abundance of PAHs in marine environments represent a risk to aquatic organisms and ultimately to humans (through fish and shellfish consumption), there is a constant need for their characterisation and quantification. The monitoring of PAH presence in the aquatic environment is therefore a world-wide activity. Since some of these compounds are well known carcinogens and mutagens, this contaminant class has been generally regarded as high priority for environmental pollution monitoring. In fact, the European Union included these pollutants in the list of priority hazardous substances for surface waters in the Water Framework Directive 2000/60/EC. There are various environmental monitoring methods that may be used in order to assess risks of PAH contamination and to classify the environmental quality of ecosystems. Among those, biological effect monitoring is defined as the exposure and effect assessment by determining the early adverse alterations (i.e biological markers) that are partly or fully reversible in selected organisms.

PAH metabolites have high affinity to nucleic acids (DNA) and proteins, which may result in adduct formation. This has been shown to be the case for human serum albumin, which is predominantly alkylated at histidine146 by diol epoxides of fluoranthene and benzo[a]pyrene. It is highly likely that the same type of mechanism is operating in animals and fish. The formation of adducts may result in reduced or impaired function of genes and proteins.

At present, new indicators of PAH pollution (related to oil production) in fish in the form of expressed proteins affected by these chemicals in the marine environment (i.e. by formation of PAH-protein adduct(s)) are under development.

The approach that will be presented aims to provide protein markers that can track the source of PAH contamination in marine environments through the identification of PAH adducts in various tissue of biological fluid of marine organisms.

AN7

Kartlegging av eksponering for Dieseleksos i Norsk arbeidsliv – hva er dieseleksos og hvordan kan vi måle dette?

Yngvar Thomassen

Statens arbeidsmiljøinstitutt (STAMI)

Dieseleksos dannes i forbrenningsmotorer med diesel som drivstoff innen transport, anleggsnæringer, industriell virksomhet og annen virksomhet hvor kjøretøy, maskiner og arbeidsutstyr benyttes. Dieseleksos består av en meget kompleks blanding av forskjellige kjemiske forbindelser og sammensetningen er avhengig av motorenes tilstand, driftsbetingelser og etterbehandling av eksosen (katalyse/filter) før utslipp. Siden partiklene i dieseleksosen i motsetning til gass/dampfasen består av relativt stabile forbindelser med lang nedbrytningstid benyttes disse i stor grad som markør for dieseleksos. Typisk sammensetning av partikkelfraksjonen er 40-60% elementært karbon og resten av den partikulære fasen består av kondensert uforbrent drivstoff. Bestemmelse av elementært karbon (EC) i luft anvendes derfor internasjonalt som en eksponeringsmarkør for dieselavgasser både i det ytre og indre miljø. For kartlegging av mulig eksponering for dieselavgasser er det også vanlig at både organisk karbon (OC), karbonmonoksid (CO) og nitrogendioksid (NO_2) bestemmes i tillegg til massen av partikulær forurensning. Dette er nødvendig for tolkning av resultatene.

I arbeidslivet vil en oppleve at forurensningen av arbeidsatmosfæren for elementært karbon kan ha forskjellige kilder. Ved utvinning av kull vil elementært karbon alltid være tilstede som hovedforurensningen av arbeidsatmosfæren. I industrien benyttes store mengder elementært karbon i form av koks og kull som råstoff i produksjon av metaller og legeringer. Avhengig av produksjonsteknologi inngår også elementært karbon som elektrodemateriale (for eksempel i aluminiumproduksjon).

I Norge finnes det også spesialisert industriell produksjon av karbonelektroder. Der hverken kull, koks eller andre tilsvarende karbonholdige råstoffer benyttes, vil imidlertid elementært karbon være en god markør for mengde dieseleksos. I hvilken grad EC vil kunne benyttes i de deler av norsk industri hvor andre kilder til EC i luft forekommer, er lite kjent. Selv om den primære partikkelstørrelsen til eksospartikler er <50 nm kan disse finnes i meget stor grad som større agglomerater i luft. I dieselavgasser og i ute- og arbeidsluft er det rapportert at hovedmengden (> 90%) av EC foreligger i partikler hvor den aerodynamiske partikkelstørrelsen er < 1 µm.

Dieseleksospartikler samles opp ved anvendelse av personbårne luftprøvetakere pakket med forglødete kvartsfiltre og cellulose støtteplater impregnert med natriumiodid (NaI) for oppsamling av NO_2. Bærbare luftpumper benyttes for å opprettholde en gjennomstrømningshastighet på 2 liter luft pr. minutt gjennom denne prøvetakeren. EC og OC bestemmes ved en operasjonell definert termo-optisk metode. Denne analysemetoden baser seg på termisk fordampning av OC i ren heliumatmosfære med etterfølgende oksidasjon av EC til karbondioksid (CO_2). Ved hjelp av to katalysatorer omdannes alle flyktige karbonforbindelser til CO_2 og videre til metan (CH_4) som kontinuerlig registreres i analysesekvensen ved bruk av en flammeionisasjonsdetektor. Kalibrering av instrumentet utføres ved innføring av en sertifisert mengde metan i hver analysesekvens. Fra et 25mm

kvartsfilter kan kun en bestemmelse utføres. Riktighet av bestemmelsen av totalkarbon (OC+EC) utføres ved bestemmelse av karboninnholdet i kjente mengder sukrose. Avviket i gjenfinning av kjent mengde totalkarbon er typisk < 10%. Bestemmelsesgrensene for henholdsvis OC og EC varierer mellom 5-10 µg og 1-2 ng per filter (3xSD av blindfiltre).

NO2 i luft vil reagere med NaI i gassfilteret til ikke flyktig NaNO2 som ekstraheres fra filteret sammen med NaI med ionebyttet vann. Vannfasen analyseres ved ionekromatografi for NO2-. Bestemmelsesgrensen for metoden er < 3µg per filter (3xSD av blindfiltre).

AN8

Korleis kan vi vite om sjømaten er trygg? Risikovurdering, biologisk variasjon og måleusikkerheit

Amund Måge, Arne Duinker, Sylvia Frantzen, Helge Hove, Kåre Julshamn, Tanja Kögel, Bente Nilsen og Stig Valdersnes

Avdeling Trygg og sunn sjømat, Nasjonalt institutt for ernærings- og sjømatforskning (NIFES), Postboks 2029, 5817 Bergen

Norge er verdas nest største eksportør av sjømat etter Kina og eksporterte rundt 2,3 millionar tonn sjømat til ein verdi av drøye 61 milliardar norske kroner i 2013. Det er også eit relativt stort innalands forbruk av sjømat både frå handel og frå sjølvfiska mat gjennom fritidsfiske.

At sjømaten skal vera trygg er eit sjølvsagt krav og kravet til dokumentasjon har auka jamt sidan 1990-talet. I dette innlegget presenterer vi det totale overvakingsregimet NIFES har vore med å byggje opp saman med blant anna Mattilsynet, Havforskingsinstituttet, FHF-fondet og Nærings– og Fiskeridepartementet. Grunnlaget for programmet ligg i prøvetakingsplanar, prøvetaking, prøvebehandling, analyse og risikovurdering.

For oppdrettsfisk som utgjer rundt ein tredel av norsk sjømat i volum er prøvetaking og analyse i stor grad underlagt felles regelverk for all animalsk matproduksjon. Minimums prøvetakingsregime er ein prøve per 100 tonn fisk/kjøtt lagt i lovverk (EU 96/23). Her inngår også krav til analysemetodar og rapportering.

For villfisk fins det ikkje noko tilsvarande regelverk. Samstundes er det mykje større grad av variasjon i den villfanga sjømaten. Blant anna er talet på artar som vert fangsta mykje større enn talet på artar oppdrettsfisk, over 50 norske artar er i sal og endå fleire vert fangsta til sjølvbruk. Det er også mykje større geografisk variasjon og større variasjon i størrelse på fisken.

For villfisken har NIFES valt å satsa på ein kombinasjon av stikkprøvebasert prøvetaking av få prøvar for enkelte artar, med ein mykje meir omfattande prøvetaking og analyse for dei artane som vi har vurdert som heilt sentrale eller som har hatt ein spesiell risiko for å kome over grenseverdi. Difor har vi til no utført seks omfattande basisundersøkingar på til saman fem artar. Dette gjeld torsk, sei, makrell, sild (to ulike stammer) og blåkveite. Her vert prøvetaking fordelt over ulike sesongar og i store delar av utbreiingsområda samt at ein prøver å få med spreiing i størrelse.

Analysane som vert prioritert er for miljøgifter der det er etablert grenseverdiar i form av øvre grenser eller der vi trur det kan kome grenseverdiar. Dette har for sjømat vore for metalla kvikksølv, kadmium, bly, tinn og arsen samt for dei organiske miljøgiftene dioksin og dioksinliknande PCB, ikkje-dioksinliknande PCB, bromerte flammehemmarar (PBDE) og polyaromatiske hydrokarbon (PAH).

Ein del sentrale problemstillingar i skjeringspunktet mellom analytisk kjemi og biologi er: kor god kvantifiseringsgrense (LOQ) må og bør vi oppnå, kor stor kjemisk usikkerheit må og kan vi akseptere, kva er ekstra utfordringar i høve til kjemiske analysar når grenseverdiar vert oppgjeven som sum av enkeltkomponentar og vi skal summere enkeltmålingar? Det siste gjeld til dømes for dioksin og PAH. Her vert også bruken av Upperbound LOQ som skal brukast for summering av dioksin vesentleg.

Dei analytiske data vert diskutert og sett i samanheng med risiko for å verta eksponert for høge verdiar av miljøgifter eller risiko for å fangsta sjømat over grenseverdi … eller for å eta for lite sjømat.

AN9

Erfaringer og resultater fra 14 år med internasjonale ringtester for persistente organiske miljøgifter i mat

Nanna Bruun Bremnes

Folkehelseinstituttet, Divisjon for miljømedisin, Avdeling for miljøgifter –kilder og risiko, Postboks 4404 Nydalen, 0403 Oslo

Persistente organiske miljøgifter (POPs) som polyklorerte dibenzo-p-dioksiner (PCDDs/PCDFs) og polyklorerte bisfenyler er distribuert globalt og praktisk talt i alle deler av miljøet. De kan utgjøre en vesentlig helserisiko for mennesker og dyr, og kan også forårsake skadevirkninger på miljøet.

For å begrense mennesker og dyrs eksponering for POPs gjennom næringsmidler er det i mange land, blant annet i EU og i USA, krav til overvåkning av disse miljøgiftene i mat og fôr. Det er derfor behov for laboratorier verden over som kan bestemme disse miljøgiftene ved lave konsentrasjoner. Laboratoriene er ofte pålagt å være akkrediterte i henhold til ISO-standarder og må vise sin kompetanse gjennom deltakelse i ringtester.

Divisjon for miljømedisin ved Folkehelseinstituttet har siden år 2000 arrangert årlige internasjonale ringtester for POPs i ulike matvarer. Vi har på denne måten kunne tilby et verktøy for kvalitetssikring av analyseresultater, og har samtidig hatt en unik mulighet til å studere laboratorienes kompetanseutvikling innen analyse av disse forbindelsene.

Jeg vil her oppsummere resultatene og erfaringene våre fra 14 år som arrangører av ringtester for POPs i næringsmidler.

AN10

Consequences of using pooled versus individual samples for designing environmental monitoring sampling strategies.

Sara Danielsson

Naturhistoriska riksmuseet, Stockholm

Choosing an appropriate sampling strategy for chemical analysis within environmental monitoring includes the important decision of whether to sample and store individual or pooled samples. This choice impacts on future analyses from Environmental Specimen Bank samples. A number of advantages exist to support using either individual or pooled samples for temporal trend studies. However, it is important to know the total and analytical variance to be able to design the best sampling strategy. Statistical power in temporal or spatial studies is determined by the random/unexplained sample variation. The relationship between chemical analytical error and other sources of variation, as well as the cost for collection, preparation of samples and chemical analysis, will determine the number of individuals in each pool, and the number of pools that should be analysed to achieve high cost efficiency and good statistical power.

In this presentation I will show an example, based on realistic measures of variation from ongoing Swedish monitoring of contaminants in marine biota, where the above mentioned components have been considered in order to design a cost-efficient and statistically sound sampling strategy.

AN11

Assessing competence in the laboratory

Lorens P. Sibbesen

Training & Consultancy for laboratories, DK

Abstract mangler

AN12

Analyse av fosfor i turbide vannprøver – Spesifikasjon av krav til analysemetode

Anne Falk Øgaard og Eva Skarbøvik

Bioforsk Jord og miljø, Ås

Bioforsk rekvirerer en stor mengde vannanalyser for bestemmelse av partikler og næringsstoffer i vann. Resultatene inngår i overvåkningsprogram og forskning. Næringsstoffene fosfor og nitrogen brukes blant annet som støtteparametre for å vurdere økologisk tilstand i vannforekomster i forbindelse med gjennomføringen av vannforskriften. Overvåkingsdataene inngår i lange tidsserier, noe som understreker betydningen av at en rekvirert analyseparameter blir analysert på samme måte hver gang. Erfaring har vist at skifte av laboratorium i et overvåkningsprogram kan gi uventede og betydelige «hopp» i analysenivåene.

Følgende momenter gir utfordringer ved analyse av vannprøver:

-Nomenklatur. Spesielt for fosfor finnes det mange fraksjoner og nomenklaturen for de ulike fraksjonene er ikke entydig definert. Dette har spesielt gitt misforståelser om prøven skal filtreres før analyse eller ikke.

-Metodebeskrivelse. Metodebeskrivelsene kan være vanskelig tilgjengelig, for eksempel ved referanse til Norsk standard. Det er ofte uklart hva referansen refererer til. Er det ekstraksjonsmetoden eller målemetoden? Det blir heller ikke alltid gitt informasjon om modifikasjoner av analysemetoden.

-Bruk av underleverandører. Ved bruk av underleverandører kan en vannprøve bli fraktet mellom laboratorier for utførelse av ulike analyser. Ved spørsmål angående prøvebehandling (filtrering, splitting av prøven, temperatur under oppbevaring og frakt) kan det være vanskelig å få svar.

-Svar på spørsmål eller henvendelser fra laboratoriet. Disse kan værevanskelig å forstå for folk med liten erfaring i analytisk kjemi.

-Analyse av parametere som ikke er «hyllevare». Det kan være vanskelig å få analysert en ønsket fosforparameter, fordi denne ikke inngår i de kommersielle laboratorienes analyseprogram.

-Mangelfulle metoder. Analysemetodene som brukes er utviklet for andre typer vann enn turbide vannprøver og gir dermed ikke sikre svar for denne type vannprøver.

AN13

Måleusikkerhet ved sum i multikomponentanalyser

Anders Torjuul Halvorsen

Laboratorium for klinisk biokjemi, Haukeland universitetssjukehus

Måleusikkerhet er en viktig del av et analyseresultat, og en essensiell parameter for å avgjøre en metodes egnethet. Moderne analyseteknikker er ofte meget spesifikke, og det er flere vanlige rutineanalyser hvor enkeltkomponenter blir summert til et analysesvar. Foredraget vil redegjøre for den prinsipielle mellom en analyse hvor flere komponenter blir målt med én, uspesifikk måling i forhold til en analyse hvor enkeltkomponenter blir bestemt og summert. Videre vil estimering og rapportering av måleusikkerhet i sum av multikomponenter bli gjennomgått, samt diskusjon rundt praktiske problemer rundt angivelse av måleusikkerhet for en multikomponentanalyse.

AN14

How to decide if a method is fit for intended use: The Fitness for Purpose of Analytical Methods: A Laboratory Guide to Method Validation and Related Topics

Lorens P. Sibbesen

Training & Consultancy for laboratories, DK

Abstract mangler

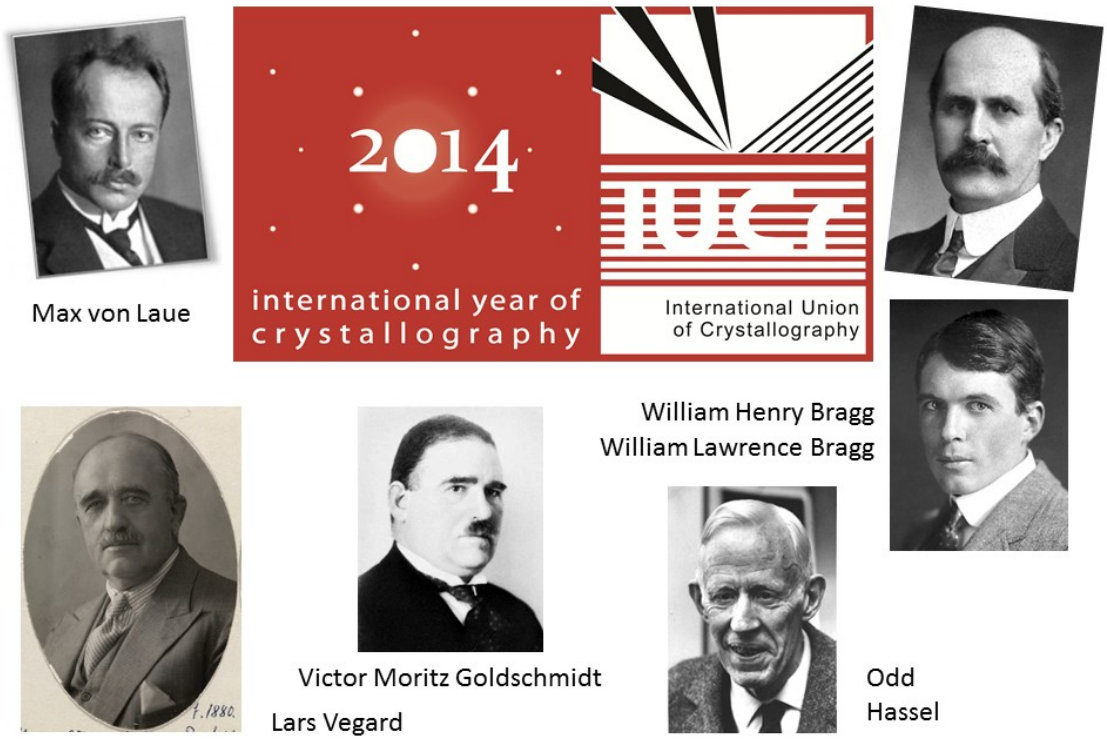
HI - Kjemiens historie

HI1

Norsk krystallografi gjennom hundre år.

Carl Henrik Gørbitz

Kjemisk institutt, Universitetet i Oslo



2014 er av FN erklært som "The International Year of Crystallography" (IYCr2014) som en markering av 100-års jubileet for røntgendiffraksjon representert ved nobelprisen i fysikk til Max von Laue i 1914 etterfulgt av William Henry Bragg (faren) og William Lawrence Bragg (sønnen) året etter. Laue påviste (eller snarere hans assistenter Walter Friedrich og Paul Knipping etter anvisning fra Laue) diffraksjon fra krystaller i 1912. Senere har det fulgt en lange rekke viktige oppdagelser. Hva var de, og hvordan ble de mottatt i sin samtid? I dette foredraget blir det gitt en kronologisk gjennomgang av banebrytende arbeider på den internasjonale arena fra de første strukturbestemmelsene utført av W. L. Bragg i 1913 (bl.a. ZnS, diamant og NaCl) til de nyeste studiene av proteinkomplekser basert på røntgen fri-elektron lasere (XFEL). I perioden har strukturkjemien hatt en sterk posisjon i Norge, der flere markante personer har satt sitt preg på forskningen ved våre universiteter. Disse vil bli viet spesiell omtale, med fokus på de problemstillingene som har vært sentrale innenfor ulike tidsepoker.

HI2

Rekonstruksjon av destillasjon på 1500-tallet

Fredrik M. Kirkemo

forhenv. Kjemisk institutt, NTNU

I 1557 publiserte den daværende stadsfysikusen i Frankfurt, Adam Lonicer (1528 - 1586), en urtebok som ble svært populær i sin samtid [1]. Urteboken er rikt illustrert med vakre tresnitt og beskriver både planter og dyr, men også destillasjonsteknologien som ble anvendt for å fremstille medisiner. Boken kan derfor betraktes både som et oppslagsverk om planter og dyr, som en farmakologi og som en håndverksbok om destillasjon. De flotte illustrasjonene og den øyensynlig store detalj-rikdommen dannet inspirasjonen til en fullskala rekonstruksjon av destillasjonsprosesser fra 1500-tallet. Dette prosjektet har vært gjennomført som en masteroppgave ved Institutt for kjemi ved NTNU, som en del av det tverrfaglige Mubil - prosjektet (museum og bibliotek - et digitalt laboratorie) [2].

Med hjelp fra spesialiserte håndverkere fra universitetets verksteder ble det rekonstruert en ovn, utstyr samt det glassutstyret som behøvdes for å reprodusere renessansens destillasjonsteknologi.

Målet med rekonstruksjonen var å undersøke utstyret og teknologiens effektivitet, målt med moderne metoder, samt å utforske synergieffekten av å arbeide med teksten parallelt med den faktiske rekonstruksjonen. Rekonstruksjon av historisk utstyr og eksperimenter i alkymi og kjemi har, som metodologi, vist seg nyttige i flere nyere studier [3], men har i større grad vært anvendt i studier av metallurgisk alkymi enn iatrokjemisk alkymi [4].

Analysene av det rekonstruerte utstyret viser at noen hypoteser om utviklingen av destillasjonsteknologi bør revideres.

Referanser

1. Urteboken finnes tilgjengelig digitalt på http://www.ntnu.no/ub/spesialsamlingene/ebok/kreuterbuch.html
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HI3

Organisk kjemi i 1830

Ragnar Bye, Berit Smestad Paulsen og Bjørn Pedersen,

Farmasøytisk og Kjemisk institutt UiO

Jørgen Gløersens notater fra professor Jac Keysers forelesninger i den organiske kjemi i 1830 har blitt oppbevart på Nasjonalbiblioteket lenge, men vi ble klar over dem først da kartotekkortene i Håndskriftsamlingen ble digitalisert og lagt ut på nettet. Notatene er skrevet med gotisk håndskrift som vi har fått transkribert av Marianne Kern. Marianne er ikke kjemiker så vi har gjennomgått og gjort endringer i teksten der Marianne tydeligvis har misforstått enkelte kjemiord.

Gløersen var 24 år da han skrev disse notatene. Han tok Eksamen artium i 1826, anneneksamen (Ex. Phil.) i desember 1827 og medisinsk embetseksamen i mai 1833. Til anneneksamen hadde han bl. a. blitt eksaminert av Keyser i naturlære dvs. fysikk og kjemi. Det betyr at disse forelesningene Keyser holdt, må være et avansert kurs i organisk kjemi for medisinerstudenter og apotekerlærlinger som bygget på det de hadde lært tidligere.

Berzelius hadde publisert sin bok i organisk kjemi tre år før [1]. Han, og andre kjemikere den gang, trodde at organiske stoffer bare kunne syntetiseres av en levende organisme og at slike stoffer ble syntetiseres i spesielle organer. Derav navnet organisk kjemi. Notatene viser at Berzelii bok har vært kjent av Keyser, men bemerkelsesverdig er at de kjemiske formler gitt av Berzelius ikke er gjengitt i notatene.

Den organiske kjemi som presenteres i Gløersens forelesningsnotater er kjemi knyttet til planter og hvordan man kan fremstille stoffer fra planter. Mye av det som er skrevet er vanskelig å forstå for oss i dag. Vi har derfor lagt til mange, forhåpentligvis oppklarende kommentarer til både kjemien og botanikken slik at dagens lesere kan forstå hva Keyser foreleste for Gløersen den gang i 1830.

Planen var at dette arbeidet skulle vært ferdig i tide til dette landsmøte, men det rakk vi ikke. Vi håper at et hefte om Gløersens notater med våre kommentarer kan foreligge til jul i år.

Referanse

1. J.J. Berzelius: Lärbok i organiska kemien. (1827) Eget forlag.

HI4

Tidsskriftet Kjemis historie fra 1904 til 1959

Bjørn Pedersen

Skolelaboratoriet, Kjemisk institutt UiO

2014-årgangen av tidsskriftet Kjemi kalles årgang 74, men egentlig burde det ha vært årgang 111. Det skyldes at dagens nummeringen starter i 1941 som første årgang kalt Tidsskrift for kjemi, bergvesen og metallurgi. Det avløste Tidsskrift for kjemi og bergvesen som kom i 20 årganger fra 1921. Det avløst på sin side Tidsskrift for kemi som kom i 17 årganger fra 1904. Så vi kan si at tidsskriftet har kommet i tre serier: 1. serie fra 1904 til 1920, 2. serie fra 1921 til 1940 og 3. serie fra 1941 til i dag.

Skolelaboratoriets samling av tidsskriftene fra 1904 til 2014. Serie 1 nederst til venstre og serie 2 nederst til høyre. Resten er tidsskriftene i serie 3 (foto: Truls Grønneberg).

Jeg vil begrense meg i foredraget til første halvpart av perioden dvs fra 1904 til 1959 – 55 årganger. I 1959 var jeg ferdig med studiene og meldte meg inn i Norsk Kjemisk Selskap. Siden har jeg fått tidsskriftet og lest hvert nummer.

Første nummer i 1904 het ikke Tidsskrift for kemi, men Pharmacia, Tidsskrift for kemi og farmaci. Det var utgitt og redigert av Eivind Koren (1869-1920). Han var utdannet apoteker, men konsentrerte sitt liv om tidsskrifter og foreninger for kjemi og farmasi. I 1915 ble tidsskriftet organ for Norsk Kemisk Selskap, gruppe i Polyteknisk forening som samme år hadde skiftet navn fra Kjemigruppen i polyteknisk Forening (P.F.).

Jeg vil i foredraget plukke ut høydepunkter fra tidsskriftet og beskrive de lange linjer i tidsskriftets historie.

UN - Kjemiundervisning

UN1

Kjemikalier og avfallshåndtering i skolen.

Brit Skaugrud

Skolelaboratoriet, Kjemisk institutt, Univ. i Oslo

Farlige kjemikalier brukes både i grunnskolen og i videregående skole, i kjemi undervisningen i naturfag og i programfag. Nettstedet Kjemikalier i skolen som er en veileder skrevet spesielt for lærere, skal gi kunnskap om regelverket som gjelder for håndtering og oppbevaring av farlige kjemikalier som brukes i skolen og være et verktøy for å få orden på kjemikaliene. Men hva skjer med kjemikaliene etter bruk? Hva produseres egentlig av farlig avfall på skolene og hvordan skal dette avfallet håndteres? Hva må lærere vite om regelverket knyttet til farlig avfall og hva trenger de av verktøy for å håndtere farlig avfall på en trygg måte? Foredraget skal gi svar på disse spørsmålene.

UN2

Organisk kjemi - hvordan få elever interessert i faget.

Yngve Stenstrøm

Institutt for kjemi, bioteknologi og matvitenskap, NMBU, Ås

Realfagsatsingen som myndighetene har satt i gang over mange år er vel kjent for de fleste. I praksis går jo denne ut på at man skal få ungdom interessert i realfag på tidlige alderstrinn slik at man får mange til å ta utdannelse innen disse fagene. Hvor vellykket dette har vært i praksis kan nok diskuteres, men det som er helt sikkert er at dersom man ikke får barn og ungdom interessert i dette på et tidlig tidspunkt, så er de tapt med tanke på et universitets- eller høyskolestudier. Derfor er det viktig ikke bare å vekke nysgjerrighet og interesse så tidlig som mulig, men også å holde på denne interessen gjennom oppveksten til en ferdig utdannet realfagskandidat. Så hvordan kan man gjøre dette?

Noe fasitsvar finnes neppe. Og metodene vil selvsagt også variere avhengig av fagområdet. Men av egen erfaring både i undervisning av studenter og ved mange skolebesøk og besøk ved utstillinger, så er det ingen tvil om at såkalte knallforelesninger vekker interesse for kjemi. Imidlertid er det lett å gå i den fellen at man bare lager show med smell, lys og farger, men uten å knytte dette til annet enn at ”dette er kjemi”. Da er det nok populært der og da, men vil også være fort glemt. Derfor er det viktig å knytte forsøkene til noe gjenkjennbart og hverdagslig. Og helst med en mer eller mindre popularisert forklaring (det vil selvsagt

avhenge av årstrinnet og nivået på tilhørerne). Kan man i tillegg lage en liten historie rundt dette, så er det også lettere å huske og å kjenne igjen historien og kjemien bak dette. Som kjemiker er derfor utfordringen å identifisere "kjemikaliene" rundt seg, og da definert i videste forstand. Eksempler på slike kjemikalier er fett, sukker, proteiner, såper, diverse matvarer generelt, plastmaterialer, treverk etc. etc. I praksis er det jo absolutt alt vi omgir oss med. Ved å ta utgangspunkt i slike ting kan man dessuten ta bort en del myter om at "alle kjemikalier er farlige". I tillegg kan man fortelle at mange av forsøkene med disse hverdagskjemikaliene kan man faktisk selv utføre hjemme om man vil. Så om man gir en liten oppskrift på hva man kan gjøre, vil det være enda bedre.

I foredraget vil jeg fokusere på slike eksempler og også gi noen få eksempler på dette.

UN3

Kan hydrogen bære energi?

Per Odd Eggen

Skolelaboratoriet, NTNU, Trondheim

Hva betyr læreplanmålene "….elevene skal kunne forklare rollen til hydrogen som energibærer i fotosyntese og celleånding", og "…. gjøre rede for struktur og egenskaper til … ATP?" Dette temaet kom inn i læreplanen i 2006 og innlegget vil drøfte utfordringer og muligheter som ligger i disse læreplanmålene. Er det mulig å se dem i sammenheng med resten av kjemifaget og på tvers av faggrensene?

Biokjemidelen av pensum kan være til nytte på minst to måter:
Den kan fungere som spesifikke eksempler på tema som er gjennomgått i Kjemi 1 og Kjemi 2 og dermed fungere som en slags repetisjon. Virkemåten til ATP kan i hovedsak gå ut på å drøfte bindinger, bindingsenergier og termodynamikk.

Når hydrogen virker som energibærer, dreier det seg om spontane og ikkespontane redoksreaksjoner der "endepunktene" er spalting av vann og dannelse av vann. Reaksjonene i elektrontransportkjedene kan virke svært kompliserte, men de kan også være egnet til å repetere grunnleggende prinsipper.

For elever som tar biologi i tillegg til kjemi, kan de nevnte læreplanmålene gi en dypere forståelse av de kjemiske prosessene i fotosyntese og celleånding. Dette gjelder egentlig alle elevene, siden fotosyntese, celleånding og ATP også er tema i naturfaget.

UN4

Nanopartikler

Ola Nilsen

Kjemisk institutt, Univ. i OSlo

Nanoteknologi skal være vår mirakelkur for alt. Hva er egentlig nanoteknologi, og hvorfor fungerer ting annerledes når det blir smått?

Naturen er en overlegen produsent av nanomaterialer, men likevel ropes det varsko når produksjonen bringes inn i en labb. Hva er det som gjør oss usikre på hvor dette kan ende?

KM - Kvantekjemi og modellering

KM1

Orbital transformations for the localization of non-orthogonal molecular orbitals

Ida-Marie Høyvik[a], Poul Jørgensen[b] and Jeppe Olsen[b]

[a]Dept. of Chemistry, Norwegian University of Science and Technology, Norway
[b]Dept. of Chemistry, Aarhus University, Denmark

Spatially localized Hartree-Fock molecular orbitals have become an important tool in the quest for low scaling post Hartree-Fock methods. The local orbitals enable us to exploit the local nature of electron correlation to reduce computational complexity, which is essential for being able to do calculations on large molecular systems. When dealing with orthogonal Hartree-Fock orbitals, the orbital locality is limited by nodal structure required to fulfill the orthogonality constraints. Hence, there may be a gain in locality by allowing the molecular orbitals to be non-orthogonal, i.e., by relaxing our constraint on the molecular orbital overlap matrix (the metric). We consider three orbital transformations for localizing non-orthogonal molecular orbitals; a metric-conserving transformation, a metric-breaking transformation, and a transformation which conserves the trace of the metric. All of the above transformations conserve the Hartree-Fock optimization condition, and are used to generate spatially more compact Hartree-Fock orbitals for the use in post Hartree-Fock calculations.

KM2

Redox processes of different transition metal triphenyl corroles and their impact on corrole aromaticity.

Hugo Vazquez Lima

University of Tromsø

The triphenylcorrole (TPC) is the simplest triarylcorrole and several metal-corrole complexes have been characterized. We used previously reported redox potential values from 9 TPC compounds (MX[TPC] where M = Mn, Fe, Co, Cu, Ag, Pt or Au and X = C_6H_5, C_6H_4CN, C_6H_5CN, Cl or $P(C_6H_5)_3$) to test the ability of 5 DFT functionals to reproduce their first oxidation and first reduction potentials. It was found that BP86 and B3LYP have the best estimation of the experimental data and that most of these redox processes take place at TPC,

only 2 out of 16 happen at the metal center. Additionally, it was noticed that TPC suffers geometrical rearrangements to avoid metal-centered redox processes while oxidized from aromatic $[TPC]^{3-}$ to antiaromatic [TPC]-. The geometrical distortions were further analyzed and identified in a set of 110 crystallized corroles. Trends in corrole geometrical patterns and its correlation with aromaticity were established.

KM3

Local electric fields and ionization potentials in dielectric liquids.

Nazanin Davari[1], Christopher D. Daub[1], Per-Olof Åstrand[1], and Mikael Unge[2]

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Insulating liquids are often used as a dielectric barrier between two electrodes in high-voltage equipments and may suffer a breakdown in high electric fields. Breakdown happens when a conductive plasma channel, a streamer, is created in the high field regions which propagates through the barrier and bridges the gap between two electrodes. This phenomenon is influenced by the electric field-dependent molecular properties of the insulating liquid. The ionization potential decreases with increasing field while the excitation energies remain almost constant in comparison to the ionization potential [1-3]. At an excitation energy, the response of the local field to the external electric field increases abruptly, and local field factors have been calculated for liquid benzene. These changes could affect the number of free electrons at the location of high electric fields so that the propagation of streamers can be altered in dielectric liquids.

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KM4

Molecules in strong magnetic fields: non-uniform fields

Erik Tellgren[a]

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I will discuss recent work on ab initio (primarily Hartree-Fock level) methods for molecules in finite magnetic fields, with focus on non-uniform magnetic fields. Non-uniform magnetic fields give rise to novel static response properties, e.g. molecular anapole moments and anapole susceptibilities. Numerical results illustrate a connection between anapole susceptibilities and chirality as well as the dramatic improvement in basis set convergence offered by London atomic orbitals [Tellgren & Fliegl, JCP 139:164118, 2013]. Because spin symmetry is lost, this is also a case where a full treatment requires 2-component methods despite the lack of relativistic effects.

KM5

Coupled-cluster theory for molecules in strong magnetic fields

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In astrochemistry, very strong magnetic fields play an important role. Fields of about 100 T to 100 kT arise around white dwarfs while in neutron stars the fields are even higher (1-100 MT). The interpretation of observed spectra is hampered by the fact that in laboratory measurements magnetic fields can only be produced to up to about 50 T for static fields and to 1000 T in destructive pulse experiments.

Therefore, theoretical investigations may help in understanding the substantial influence of strong magnetic fields on the energies and properties of molecules. Usually, magnetic field-dependence in quantum-chemical calculations is treated via a perturbative approach using a Taylor expansion around the field B = 0. Employing a more rigorous treatment, however, enables the study of molecules in finite fields of arbitrary strength and led to findings showing distinctly modified chemical properties in very strong fields such as a paramagnetic-to-diamagnetic transition for closed-shell molecules [1] and a new paramagnetic bonding mechanism in diatomics [2].

In this work, coupled-cluster capabilities are introduced to the LONDON program which treats the magnetic field in a non-perturbative manner and uses London orbitals (GIAOs) in order to ensure gauge-origin invariance. As Full-CI results indicate an increasing single-reference character for higher field-strengths, the performance of truncated coupled-cluster approaches is expected to be advantageous. We will present results for energies and magnetizabilities, thereby investigating the influence of field-strengths, electron-correlation, and the use of GIAOs.

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KM6

Modeling of the adiabatic connection under the influence of external magnetic fields

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When studying electronic systems, the density is a central quantity. It is of particular interest for magnetic properties, where the diamagnetic part is solely determined by the ground state density at zero magnetic field, and only the paramagnetic part explicitly depends on the external magnetic field. In other words, as long as a method gives a considerably wrong density, there is little point in fixing the more elaborate electron correlation entering the paramagnetic part of the properties, since that one will be prevailed by the error in the diamagnetic part due to the wrong density.

We therefore study the electron density obtained with several density functionals, and compare the error made with respect to the density obtained with Coupled Cluster, in particular CCSD(T). Special emphasis is put on the comparison with Hartree-Fock.

We show that, in general, the error of the total density integrated over whole space is smaller for the DFT calculations, which is reasonable, since integrals like energies and properties is what the DFT functionals are optimized for. However, pointwise, there exist regions where DFT performs considerably worse than Hartree-Fock, in particular near the nuclei. Since the total density always integrates to the total number of electrons, a huge error in small regions like the intermolecular axis must result in a corresponding error in outer regions, which in the end also effects the calculation of properties.

This is an important starting point for further work on the optimization of DFT functionals. Apart from the density, we also study the NMR shielding, and analyze diamagnetic and paramagnetic part separately.

KM7

High order geometric derivatives in quantum chemistry calculations: challenge, solution and implementation

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The evaluation of high order geometric derivatives presents great challenge in practical calculations. Both the use of processors and memory need to be considered carefully for an efficient evaluation of the large amount of high order geometric derivatives, in particular in the case of large molecules. In the current contribution, I will address this problem by generating and addressing any non-redundant and non-zero geometric derivative on the fly. The proposed scheme here allows one to calculate all geometric derivatives effectively by using a large number of processors. Moreover, a two-level parallelization (distribution of geometric derivatives and calculations of individual derivatives/integrals) and an implementation of distributed-memory matrix (for instance through ScaLAPACK) will make it possible to calculate high order geometric derivatives of large molecules.

KM8

Why is Dithizonatophenylmercury(II) photochromic? An electronic structure study of the mechanism

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The color of dithizonatophenylmercury(II) (DPM) in non-polar solvents, e.g. in hexane, changes reversibly from orange to blue under illumination with blue light [1–3]. This photochromic phenomenon corresponds to a photoisomerization around a ground-state C==N double bond. We have performed calculations employing the DFT, TDDFT, CC2 and CASSCF electronic structure methods in order to answer the following questions: (i) Which electronic states are involved in the photoreaction? (ii) Which nuclear degrees of freedom, in addition to the reactive C==N bond, are activated in this process? (iii) Can we identify one or more conical intersections that induce internal conversion processes? (iv) Do spin-orbit

coupling effects triggered by mercury play a role in the rearrangement? In this talk, preliminary results will be presented. In particular, we show that the reaction is initialized by excitation of S2 and not of S1.

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KM9

Theory-Assisted Discovery and Development of Z-Selective Olefin Metathesis Catalysts

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Traditional catalyst discovery is driven by chance and serendipity and improving the design of a catalyst usually involves costly and time-consuming experimental trial-and-error. However, little by little computational chemistry is becoming more of a guide to experiment, and this trend is transforming the way in which catalysts are discovered and developed [1]. Here we present one example in which theory has been determinant for the discovery and improvement of highly Zselective olefin metathesis catalysts. Achieving such catalysts has been a major goal in olefin metathesis for years [2], with reasonably selective catalysts being obtained only recently [3]. With the help of density functional theory calculations, we discovered that non-selective, commercially available ruthenium-based catalysts easily can be modified to become highly Z-selective by replacing one of the two anionic ligands (most often a chloride) with a sterically demanding thiolate; see the left-hand side of Figure 1 [4]. We have developed a comprehensive computational approach to improve the design of these catalysts. This approach is based on detailed insight into the metathesis mechanism and also accounts for catalytic activity and stability. Using this approach, we have reached a catalyst (2) with an unprecedented robustness, tolerating air and acids, from 1 by replacing the chloride ligand by isocyanate [5]. Further improvements include increasing the steric bulk of the aryl group (Ar) in para position of the benzene thiolate, achieving catalysts giving up to 97 % Z-selectivity in metathesis coupling reactions of common 1-alkenes (3) [6].

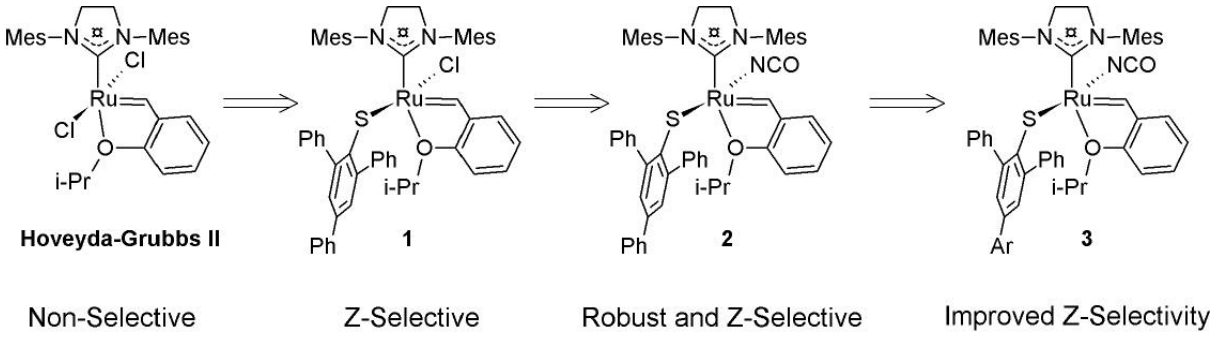

Figure 1: Evolution of Z-selective, thiolate-based ruthenium olefin metathesis catalysts.

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KM10

Asymmetric transition metal-catalyzed hydrogenation ractions: Insights into the selectivity-determining factors

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This presentation focuses on DFT studies of transition metal-catalyzed asymmetric hydrogenation reactions. We have investigated several chiral hydrogenation catalysts to elucidate their mechanistic details and the factors that govern the experimentally observed enantiomeric excesses (ee's) [1-3]. Particular focus will be on alkene hydroge-nation with iridium complexes exhibiting N,P type ligands [4]. We show that for this type of complexes, the selectivity-determining interactions between substrate and catalyst are governed by strong

CH/π type interactions (Fig.1a). Further, we provide a possible explanation for the experimentally observed temperature-dependence of the ee.[1,4] The reduced ee observed at lower temperature is not due to a change in the relative hydrogenation barriers (ΔΔG≠R-S appears unaffected by temperature), but is due to an increase in the barrier for isomerization between two isomeric substrate-catalyst complexes (minor and major, Fig. 1b), which differ with respect to the alkene-coordination mode. We further present a small set of benchmark calculations on different iridium-complexes, showing good performance of the employed computational protocol (B3LYP-D2/IEFPCM) [1].

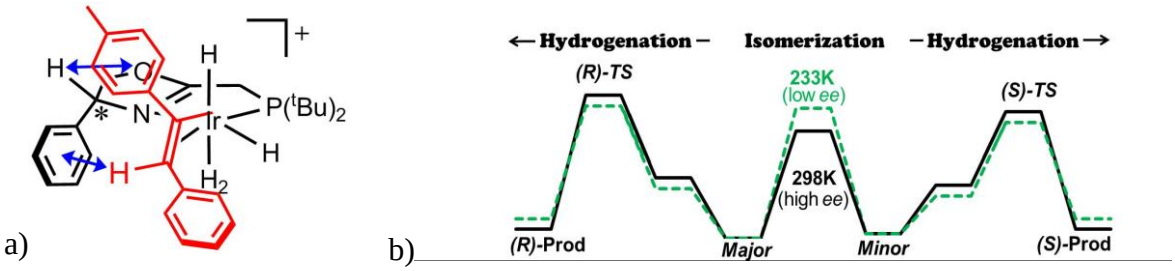

Fig. 1: a) Example of selectivity-determining CH/π interactions (blue arrows) between an alkene substrate (in red) and a chiral N,P-iridium hydrogenation catalyst (in black). b)Schematic illustration of computed energy profile. The barrier for isomerization between alkene-catalyst complexes (minor and major, differing in the alkene coordination mode) increases at lower temperature, which results in reduced enantiomeric excess (ee).

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KM11

DFT Adventures on Structure, Reactivity, Development and New Concepts

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In this talk I will present a short overview of DFT studies in close collaboration with experimental groups on the field of organometallic chemistry and catalysis. These studies focus on several topics including: 1) characterization of polyhydride iridium clusters (catalytic hydrogenation);[1] 2) mechanistic studies on catalytic cross-coupling reactions (synthesis of fine chemicals);[2] 3) unexpected products in the copper-catalysed oxidation of alkanes (activation of small inert molecules)[3] and 4) unprecedented strengthening and deactivation of ancillary ligands in transition metal complexes.[4]

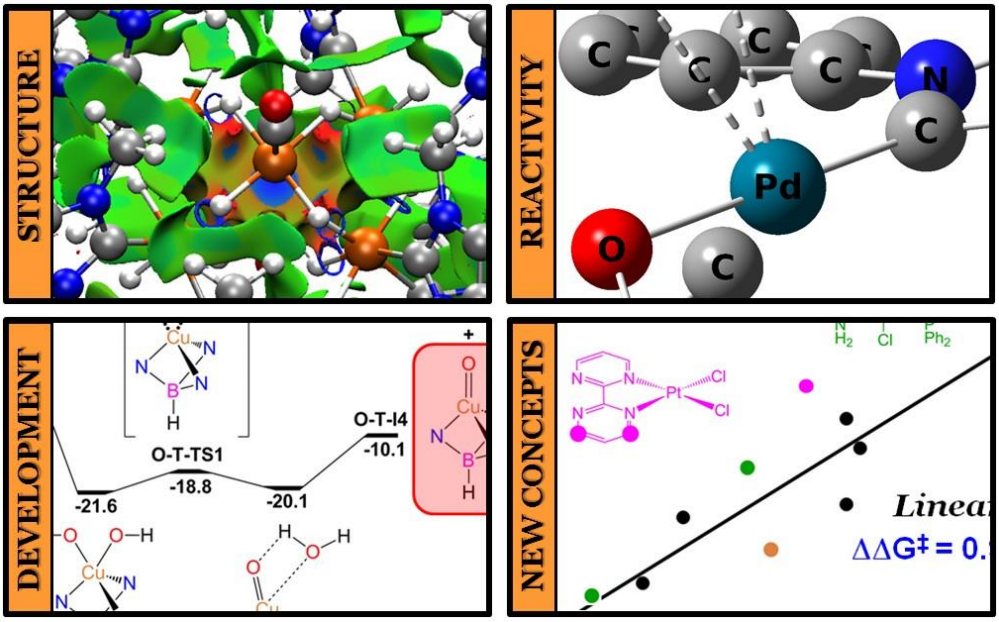

Figure: Joint theoretical-experimental projects with DFT.

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KM12

Nucleophilic substitution reactions of partially hydrated superoxide anions with alkyl halides

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The ability of a molecule to donate an electron pair to a substrate and displace a leaving group during an SN2 nucleophilic substitution reaction is strongly affected by solvent effects.Superoxide anion, O^{2-}, is an essential intermediate in the cellular processes of electron transport, including the respiration chain and photosyntheis, and plays a key role in the immune defence system of organisms. The investigatigation of the properties and reactivity of superoxide and superoxide/water clusters in the gas phase offers insight into the atmospheric chemistry of the species, and understanding of how O^{2-} reactivity is moderated by hydration.

This work investigates the gas-phase reactivity of bare O^{2-} and water clusters containing it, $O^{2-}(H_2O)_n$, in substitution reactions with CH_3Cl, CH_3Br. Besides studying the degree of hydration on reactivity, it was of interest to investigate the effect of the leaving group and to examine the nature of the products. The reactions were studied using mass spectrometry.

In order to help assisting the interpretation of the data, we have conducted quantum chemical calculations of the selected reaction profiles, including the identification of key intermediates and transition state structures. In addition, Born Oppenheimer direct dynamics calculations were conducted to examine the product formation in detail, with particular emphasis on the possibility of water molecule transfer during reaction.

KM13

Doing Computational Chemistry faster and bigger - opportunities for computational chemistry in the national electronic infrastructure for science

Espen Tangen [a]

[a] **Norwegian Supercomputing Centre (NOTUR), Norway**

The Norwegian Metacenter for Computational Science (NOTUR)provides the national infrastructure for computational science in Norway. Currently, computational chemistry is one of the major consumers of computer time on the national facilities.

In addition, we have indications showing that our users in average publishes in more highly ranked jornals than academic staff that not are using computational resources.

Thus, the focus of this talk would be split:

I present the national project on direct user community support for computational chemistry, both in terms of available resources, possibilities, and the need for better communication!

I also want to present oppurtunities for potential users of our services. This will include a brief presentation of the different facilites in Norway, the current list of available software and also necessary links for applying for access and user training."

KM14

Calculating transport properties from first principles: thermoelectric materials as a playground

Ole Martin Løvvik [a, b]

[a]**SINTEF Materials and Chemistry, 0314 Oslo**
[b]**University of Oslo, Dept. of Physics, 0316 Oslo**

Many devices rely on materials transport properties like electrical resistivity, heat conductivity, and the Seebeck coefficient. (Given a temperature difference, the Seebeck coefficient determines the resulting voltage between two ends of a material.) This is particularly so for nanoscale energy conversion technologies, which are likely to change radically how we generate, transport, and use energy in our daily lives. One example is thermoelectric materials, which can be used both for heating/cooling purposes through the Peltier effect or electricity production from waste heat or renewable sources through the Seebeck effect (Fig. 1).

Prediction of such transport properties is challenging, and it is only recently that electronic structure calculations have been available for calculating some of them without adjustable parameters. We are in this presentation going to look at what has been achieved so far, and what remains before reliable predictions about realistic materials can be expected.

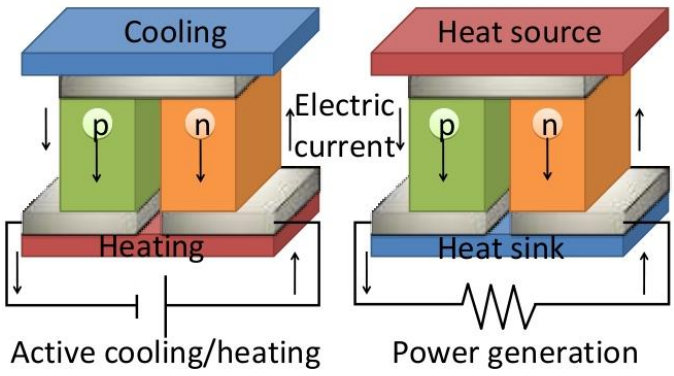

Figure 1: Thermoelectric materials can be used for cooling or heating through the Peltier effect (left) or for production of electricity through the Seebeck effect (right). Their charge carriers are either electrons (n-doped) or holes (p-doped).

KM15

Chemical structure from photoelectron spectroscopy

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In X-ray photoelectron spectroscopy (XPS) the ionization energy of inner-shell electrons is measured by means of soft, monochromic X-rays. The radiation and hence the relevant ionization energies appear on an energy scale of 100-1000 eV (104-105 kJ/mol), with an experimental energy resolution of about 0.1 eV (10 kJ/mol). Thus, the spectroscopic process appears on a much coarser energy scale than most aspects of chemical structure. Nonetheless, by combining theoretical models of the fine structure in X-ray photoelectron spectra with state-of-the-art experimental spectra, workers have been able to extract a wide range of chemical structure information from this, until recently, unexpected source. The presentation aims to exemplify and explain different mechanisms whereby photoelectron spectra may provide information on interatomic distances. In concluding, some remarks will be offered on the possible future role of XPS as a structure method in chemistry.

KM16

Computational determination of a mechanism for silicon island formation in SAPO materials

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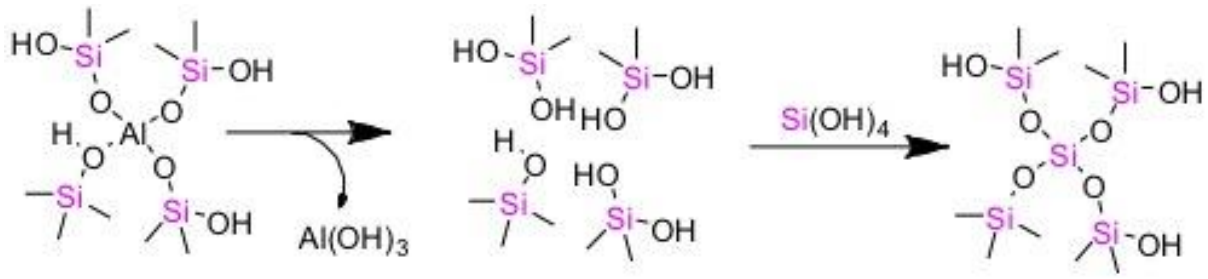

Scheme 1:Al/Si substitution

SAPOs are microporous, crystalline aluminophosphates in which some phosphorus atoms are substituted by silicon. The substitution necessitates the presence of extraframework cations; when these are protons, a solid acid results. SAPOs have important applications in catalysis. Over time, the silicon atoms move through the material, forming silica moieties called silicon islands. While a thermodynamic driving force for this process has been experimentally

established, this is undesirable from a catalytic point of view, and the mechanism for the reaction has been unknown.

Based on large-scale periodic density functional theory calculations, we propose a mechanism for silicon island formation. Firstly, silicon and aluminium atoms are hydrolyzed to Si(OH)4 and Al(OH)3(H2O) by water molecules in four consecutive steps (Scheme 1, Figure 1). Then, P in the crystal lattice may be exchanged with Si in hydrolysis reactions involving water and Si(OH)4. While we cannot rule out other mechanisms on the basis of these results, the proposed mechanism is thermodynamically and kinetically feasible.

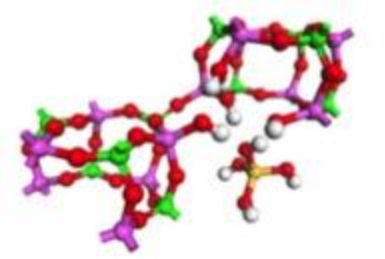

Figure 1: Si(OH)4 and hydrogarnet defect formed by 4-step hydrolysis.

Acknowledgments

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KM17

Defect properties of functional oxides from first principles

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Defect related phenomena affect, and in many cases completely determine, the functional properties of ceramics. Defect engineering for instance allows control of the ionic conductivity of ceramic electrolytes in solid oxide fuel cells, the electrical activity of semiconductors, necessary for the construction of p-n-junctions, and the critical temperature of novel high temperature super conductors. Controlling the defect properties of a material requires knowledge of its defect structure, i.e. the concentration of all defects under all atmospheric conditions, and as a function of temperature. The free energy of formation of the individual defects, which governs their relative dominance, is, however, difficult to address experimentally. In the recent decade, periodic first principles calculations have therefore proven vital in defect chemical analyses of functional ceramics as they enable investigations of the stability of individual defects. This contribution explores the ability of current first principles techniques to predict finite temperature defect structures in selected functional ceramics.

KM18

Modulation of protein function by micro-solvation effects: the puzzling case of cis-retinal binding in CRALBP

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2 Department of Chemistry and Biochemistry, University of Bern, Switzerland

In all biological phenomena involving protein-ligand interactions, solvation plays crucial effects, both in the thermodynamics and in the kinetics of binding. In this seminar, I will present how combined computational and experimental data reveal peculiar and unexpected properties of binding of cis-retinoids to cellular retinaldehyde binding protein (CRALBP) and its mutant R234W, associated to Bothnia retina dystrophy disease. Molecular dynamics simulations show that residual hydration in the large hydrophobic binding cavity plays a major role for recognition and binding of the substrates. Due to the absence of strong directional contacts, multiple conformations of the ligands inside the cavities of the different proteins are possible at room temperature for different ligands. The micro-solvation pattern characteristic of 9-cis-retinal binding in CRALBP evidenced by our simulations is responsible for a newly discovered secondary thermal isomerase activity, which may be connected to biological processes other than imaging forming.

KM19

Reaction path sampling using rare event simulation techniques

Titus van Erp

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I will discuss the QuanTIS method which is presently being developed in my group and can be viewed as a dynamical analogue of QM-MM. Just like QM-MM, QuanTIS tries to combine the best of both worlds: accurate quantum-based MD and fast classical MD simulations. However, whereas QM-MM is designed to obtain a large system size with QM accuracy, QuanTIS aims to boost the timescale, even beyond the point of straightforward classical MD.

KM20

Accurate QM/MM made cheaper: a hybrid approach to calculate polarizable embedding potentials

Maarten Beerepoot [a], Nanna Holmgaard List[b], Arnfinn Hykkerud Steindal[a], Jógvan Magnus Haugaard Olsen[c], Kenneth Ruud[a] and Jacob Kongsted[b]

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The balance between accuracy and efficiency is of central importance in computational chemistry, in particular in the calculation of accurate molecular properties at a reasonable cost. Multiscale modeling deals with this challenge by treating a central part of the molecular system (e.g. a molecular probe or the active site of a protein) with an accurate method while describing the surrounding (e.g. the rest of the protein or a solvent) with one or more approximate methods. In polarizable embedding approaches, the surrounding is modeled by a potential containing charges and polarizabilities. The most accurate and expensive way is to derive these parameters from quantum mechanical (QM) calculations for every molecule or protein residue separately. The cheapest and most approximate way is to take only atomic charges from a pre-parametrized force field such as OPLS. The objective of our study is to find a balance between accuracy and efficiency by combining QM-derived parameters for the innermost molecules with molecule-specific average parameters for the molecules further away. We will show results for optical and vibrational properties of molecules in different solvents. The approach will be extended to proteins and lipids in the future to allow for accurate and efficient modeling of vibrational and fluorescent probes in biomolecular systems.

KM21

Thermal conductivity of carbon dioxide from non-equilibrium molecular dynamics: a systematic study of several common force fields

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Carbon dioxide (CO2) has an important impact on the climate and is therefore widely studied. Huge efforts are being made, for instance to reduce emissions of CO2 to the atmosphere, by capture- and sequestration techniques. In that context, membrane separation techniques are needed, at high as well as low temperatures. Fossil-fueled power systems, natural gas processes or production of hydrogen gas includes all high-temperature separation

technologies. The thermal conductivity of CO2 is needed for process modelling in these processes[1,2].

We report a systematic investigation of the thermal conductivity of various three-site models of carbon dioxide (CO2) using nonequilibrium molecular dynamics in the temperature range 300 -1000K and for pressures up to 200 MPa. A direct comparison with experimental data is made. Three popular CO2 force fields (MSM, EPM2 and TraPPE) and two flexible models (based on EPM2) were investigated. All rigid force fields accurately predict the equation of state for carbon dioxide for the given range of variables. They can also reproduce the thermal conductivity of CO2 at room temperature and predict a decrease of the thermal conductivity with increasing temperature. At high temperatures, the rigid models underestimate the thermal conductivity.

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KM22

Divide wisely and conquer accurately: a strategy to please chemists who are notorioulsy demanding customers

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Much of the effort in Quantum Chemistry development is towards the goal of so-called chemical accuracy: energetics computed with an error within 1 kcal/mol. Larger errors can often lead to predictions – e.g. in the outcome of a reaction – which can be anything between quantitatively inaccurate (wrong yield) to qualitatively inconsistent (wrong product). In order to achieve the goal for medium and large systems (100 electrons or more) the only practical strategy so far is using Density Functional Theory with a large basis set (augmented triple-zeta or larger), often relying on a fortuitous error cancellation between the basis and the functional. An alternative to atom-centered basis functions which is currently pursued is the use of Multiwavelets[1], which allow guaranteed precision with respect to the basis set limit for energetics[2] and properties alike. By pursuing this approach the outcome of a prediction become therefore as good as the functional used, which is hence the only source of error. The Multiwavelet framework will here be presented with reference to our work[3, 4] and some recent developments in the calculation of molecular properties and a divide-and-conquer approach for larger systems.

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KM23

Molecular properties in the random phase approximationy

J. Rekkedal, K.R. Leikanger, M.F. Iozzi, S. Coriani, A. M. Teale, T. Helgaker, Thomas Bondo Pedersen

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The random phase approximation (RPA) to the electronic correlation problem has undergone a revival in the past decade in the quantum chemistry and materials science communities [1-3]. Providing a computationally a ordable and parameter-free description of dispersion interactions for metals as well as insulators, RPA is particularly attractive as an alternative to semi-empirical dispersion-corrected functionals in density-functional theory. In this talk, a Lagrangian reformulation of the RPA correlation energy will be presented, paving the way for calculations of forces and other molecular properties.[4]

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KM24

Cusp based DFT functionals

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Cusp-based correlation functionals model the density-functional-theory correlation energy by use of a model wavefunction constrained to the same density as the Kohn-Sham wavefunction, but satisfying the electron-electron cusp condition. After summing up,

expressions can be rendered as density functionals. The Lee-Yang-Parr (LYP) correlation functional is a cusp-based correlation functional, based on the Colle-Salvetti expression. We will discuss the LYP and Colle-Salvetti expressions and our efforts to rectify their shortcomings.

KM25

Optimisation problems from exact DFT

Ulf Ekström [a]

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Lieb's formulation of exact density functional theory gives rise to optimisation problems that are either constrained or non-smooth. These two complications makes the problems much harder than the ones usually encountered in quantum chemistry. I will show how non-smoothness is can be related by duality to constrained optimisation, and discuss some new algorithms developed at the CTCC in Oslo for non-smooth problems.

Finally I will discuss the geometrical interpretation of the chemical Aufbau principle, and the connection to the SCF procedure and the DIIS algorithm of Pulay.

MA - Matkjemi

MA1

GMO i maten vår – et glimt inn i fremtiden

Askild Holck, Seniorforsker

Nofima AS

Hovedpunkter

Genmodifiserte planter (GMP) benyttes til å øke produktiviteten i landbruket. Dyrkningsarealet for GMP globalt er 175 mill. hektar. De viktigste avlingene er soya (79 % av verdensproduksjonen), mais (32 %), bomull (70 %) og raps (24 %). Disse plantene har fått bygget inn ugressmiddeltoleranse og/eller insektresistens. En rekke nye genmodifiserte planter med andre egenskaper som tørketoleranse, salttoleranse, beta-carotenproduksjon og endret oljesammensetning er under utvikling.

Abstract

I år 2050 kommer vi til å være 9 milliarder mennesker på jorden. For å sikre verdens befolkning nok mat må produksjonen fordobles innen 2050. Økt produktivitet i landbruket er fortsatt nødvendig. I planteforedling benytter man en rekke strategier som gir genetiske endringer i kulturplanter og dermed gir dem ønskede egenskaper. Genteknologi er én av mange slike teknikker. Ønsket DNA føres da inn i planten ved hjelp av bakterier eller ved bombardering med små metallkuler. Resistens mot plantesykdommer og insektangrep samt toleranse overfor herbicider er den mest kostnadseffektive måten å øke produktiviteten på. De første genmodifiserte plantene (GMP) ble tilført nettopp slike egenskaper. Fra starten i 1996 har dyrkningsarealet av GMP økt voldsomt til 175,2 mill. hektar. De 5 største produsentene av GMP er USA, Brasil, Argentina, India og Canada. De viktigste avlingene er soya (79 % av verdensproduksjonen), mais (32 %), bomull (70 %) og raps (24 %). Mange GMP har flere endrede egenskaper. Andre nye GMP er under utvikling for eksempel: trehaloseproduserende ris som er salt- og tørketolerant; tørketolerant mais; golden rice som produserer beta-caroten og kan avhjelpe A-vitaminmangel i u-land; insektresistent Brinjal (aubergine) i India; tørråteresistent potet og dodre som inneholder fiskeolje. I tillegg utvikles det GMP for produksjon av medisiner (insulin), phytoremediering og biodrivstoff. GMP har oppført seg som forventet og dyrkningsarealet for GMP forventes å øke videre i årene som kommer.

MA2

Risikovurdering av GMO-produkter

Audun H. Nerland, Professor

Universitetet i Bergen

Hovedpunkter:

Foredraget vil ta for seg hvordan risikovurderinger av GMO blir utført i dag, men også sette dette inn i en større sammenheng, både vitenskapelig, etisk og politisk. Kan bruk av GMO medføre lavere risiko enn bruk av tilsvarende konvensjonelle organismer? Vil en for restriktiv holdning i forhold til GMO være uheldig for Norge i det lange løp?

Abstrakt

Ifølge den norske genteknologiloven er alle "mikroorganismer, planter og dyr hvor den genetiske sammensetning er endret ved bruk av gen- eller celleteknologi" definert som GMO, uansett hva, eller hvor mye av det genetiske materialet som er endret. Generalisering når det gjelder risikovurdering av GMO er derfor ut fra et faglig og vitenskapelig synspunkt, helt ulogisk. Risikovurderinger, både angående bruk av GMO som mat og når det gjelder miljøinteraksjoner, blir derfor gjennomført for hver enkelt GMO som blir utviklet ("case by case"). Man ser på hvilken genetisk modifisering som er gjort, og hva det har som konsekvenser for den aktuelle organismen sine egenskaper.

I svært mange tilfeller kan utgangsorganismen i seg selv ha uheldige egenskaper. Ukokte poteter, for eksempel, inneholder giftstoffer som vil være skadelig hvis man spiser for mye, og erter kan gi enkelte personer allergiske reaksjoner. Risikovurderinger blir derfor gjort komparativt. Det vil si at man vurderer om den aktuelle GMO medfører endret risiko i forhold til utgangsorganismen ("the conventional counterpart"). Det samme prinsippet gjelder også miljømessige risikovurderinger.

Et paradoks når det gjelder risikovurderinger er at definisjonen av GMO ikke nevner noe om hvorvidt de samme genetiske forandringene kan oppnås ved bruk av tradisjonelle avls/foredlings-metoder (som også kan inkludere bruk av bestråling eller mutagene kjemikalier). Logisk sett burde alle "ny-utviklede" organismer bli vurdert ut fra de genetiske/fenotypiske forandringene som har skjedd, uansett hvilken metode som er brukt for å oppnå disse forandringene.

Ved risikovurderinger av GMO burde man også ha sett det hele i en større sammenheng. Hvilken konsekvens vil det ha hvis man ikke tillater bruk av en gitt GMO? For eksempel kan alternativet til bruk av en insekts-resistent GM-plante være bruk av stor mengder pesticider.

MA3

Tradisjonell avl for bedre geitmelkskvalitet

Knut Erik Grindaker, Fagsjef

Tine FoU

En forutsetning for å øke innsatsen på anvendelse og økt bruk av geitemelk er mild og stabil kvalitet gjennom året. Tidlig på 2000-tallet var ikke dette på plass og det ble igangsatt arbeid med hovedmål å bedre denne situasjonen. Hovedproblemet var at råstoffet i deler av året var beskt og harskt. Dette skyldes i stor grad for høyt innhold av frie fettsyrer i melka, et resultat av fettspalting.

Det ble igangsatt flere prosjekter for å finne mulige tiltak for å løse problemene på råstoffsiden. Det ble et gjennombrudd når en fant sammenhenger mellom kaseingenstatus i geitene og hvor disponert melka var for fettspalting. Det ble besluttet bevisst å avle på geiter som var disponert for å produsere alfa S1-kaseinet. Det ble avlet på norske melkegeiter som hadde denne egenskapen. I tillegg ble det importert bukkesæd fra fransk Alpin-geit. Denne geiterasen er kjent for å produsere alfa S1-kaseinet samt å ha en mild smak.

Det har blitt en formidabel bedring av råstoffkvaliteten, innholdet av frie fettsyrer er redusert til en tredjedel av nivået vi hadde i 2005. I tillegg til dette har vi oppnådd bedre ystingsegenskaper i melka.

Hovedpunkter

- Bakgrunnen for avlsmessige tiltak
- Avlen hadde hovedfokus på kaseingenstatus i geitene
- Gjennomføring av avlsprogrammet
- Resultater og status i 2014

MA4

Dyrking av grønnsaker i forskjellig klima-hva betyr det for innholdsstoffene?

Gunnar Bengtsson, Seniorforsker

Nofima AS

De fleste kulturplanter går ikke å dyrke i alle klimaer, fordi de ville forgjengerne er tilpasset bestemte voksesteder. Innen områder der hver art kan dyrkes er det dog forskjeller i klima som gir forskjeller i kvalitet. Temperaturen er den viktigste faktoren, deretter kommer lys og vann, men vann er normalt ikke begrensende for grønnsaker grunnet kunstvanning. Mekanisk stress fra vind og hagl har også betydning. I nord har sollyset lavere intensitet av UV-stråling og et større forhold mellom mørkrødt og rødt lys, samtidig som lysperioden kan være opptil 24 timer. Alle disse forhold kan påvirke nivået av innholdsstoffer som bestemmer sensorisk og helserelatert kvalitet: Polyfenoler, karoteno¬ider, glukosinolater, fettsyrer, sukker, terpener, vitaminer, etc. Likevel må man alltid ta utgangspunkt i de nivåer som er genetisk bestemt i ulike grønnsaksorter. I tillegg kan sortene ha ulik respons for klimafaktorer. Variasjonen i været fra år til år kan iblant gi en større effekt på en grønnsak enn fra ulike klima innen dyrkingsområdet, f eks. mellom Nord- og Sør-Norge.

Ved tidl. Matforsk ble det forsket på kvalitet av gulrot i en nord-sørgradient. Lavere temperatur ga søtere og sprøere, men bleikere gulrøtter. Dette samsvarer med et lavere innhold av sukrose og karotener og et høyere innhold av glukose og fruktose. Både før og etter innhøsting kan mekanisk stress gi bitre gulrøtter med høyt innhold av isokumariner (6 methoxymellein etc.) og polyacetylener (falcarindiol etc.). Altfor tett pakning gir gulrøtter med emmen smak, på grunn av anaerob metabolisme. På basis av disse resultatene er det utviklet et produkt som heter Smaksgulrot.

Mange kålvekster klarer bare kjølige betingelser. I Syd-Europa kan de dyrkes om vinteren, men klarer ikke varmen om sommeren. Derfor eksporterer faktisk Norge brokkoli og blomkål til Syd-Europa om sommeren, mens en rekke kålvekster importeres derfra resten av året. Ved Nofima har vi i samarbeid med Bioforsk og NMBU nå avsluttet et prosjekt på effekter av betingelser både pre- og postharvest for kålvekster («Northern vegs», støttet av Norges forskningsråd og Fondet for forskningsavgift på landbruksprodukter). Et semi-feltforsøk på brokkoli fra Spania til Nord-Norge er gjennomført i tillegg til flere forsøk i klimakammer. Resul¬tater fra disse forsøkene, men også fra postharvest lagringsforsøk med behandling med UV-stråling og synlig lys ved ulike temperaturer, vil bli presentert. For ulike klimaer hadde brokkoli ulik tekstur, utseende og smak. Av innholdsstoffer i brokkoli ble flavonoler påvirket mest, deretter ulike glukosinolater på en kompleks måte, mens vitamin C var lite påvirket.

OM - Organisk, Makromolekyl- og kolloidkjemi

OM1

DNA-Programmed Assembly of Molecules and Materials

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The idea behind our research is to use DNA as a programmable tool for directing the self-assembly of molecules and materials. The unique specificity of DNA interactions and our ability to synthesize artificial functionalized DNA sequences makes it the ideal material for controlling self-assembly and chemical reactions of components attached to DNA sequences. We have applied these concepts to assemble and covalently couple conjugated organic molecules [1] and dendrimers [2]. Recently, we extended this to DNA templated conjugation of DNA to proteins. In our studies of DNA origami we developed a method to image chemical reactions with single molecule resolution[3] and to make a 3D DNA origami box with a controllable lid [4]. More recently, we prepared a DNA-phenylene vinylene polymer and assembled it on DNA origami for studies of electronic and optical properties. In extension of this a method for self-assembly of DNA origami and single stranded tile structures at room temperature will also be presented [5].

Schematic illustration and AFM image of poly(DNA-phenylene vinylene) on DNA origami.

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OM2

A tissue-like multifunctional 3D scaffold - Design and functionalization of resorbable matrices to adapt cell-material interactions

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The trend within tissue-engineering research is to obtain material which stimulate, optimize and control cell-material interactions. Materials that are bioactive, biomimetic, multifunctional, and degradable ought to be designed to specifically stimulate cells and biological processes in a spatial and temporal controlled manner. There are many parameters to play with, for example surface topography, hydrophilicity, the mechanical properties, scaffold design and material functionality. The number of parameters in combination with number of applications makes it important to develop a tool box for tissue regeneration, which on one hand fulfils basic requirements and on the other hand is freely combinable with what is needed in the respective clinical situation. We are developing this tool box by establishing synthesis methods and fabrication techniques.

- Synthetic biodegradable polymers are widely applied today as 3D scaffold materials in tissue engineering research because their chemical, physical and mechanical properties are predictable and extremely adjustable through variation of monomers, co-polymers, blends and architectures. However, a new generation of biocompatible and degradable synthetic polymers with various physicochemical, functional and biological properties is required to obtain scaffolds which facilitate advanced tissue engineering. We have functionalized degradable aliphatic polyesters to extend their properties and the utility of this class of materials in biomedical applications. For example, functionalized polyesters from radical ring-opening polymerizations of ketene acetals and electroactive copolymers.[1-4]
- A variety of fabrication processes to obtain scaffolds with highly porous and well interconnected pore structure have been developed; each combination of material and process has unique matrix architecture and mechanical properties. To overcome limitations such as manual intervention, use of toxic organic solvents and use of porogens and shape limitations, solid free form fabrication was introduced and fused deposition modeling (FDM) has successfully been used. An additional advantage is that the scaffolds are with this process built using layer-by-layer, raising the possibility for hierarchical design. We have used different fabrication processes over the years and it has been shown that they are biocompatible and stimulate bone regeneration both in vitro and in vivo.[4-6]

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OM3

Advanced Technical Textiles

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For thousands of years mankind uses textiles to protect us against the weather, as well as to keep us warm and dry (clothes, tents). At the same time, textiles are important for fashion reasons and as interior materials (curtains, carpets). Textile materials offer a number of advantages that make them essential for clothes as well as for technical textiles. Fabrics can be draped in many different forms - if needed thousands of times. They can be prepared to be flexible as well as inflexible. They show a certain permeability for air, vapor and liquids and textiles combine an enormous stability (especially tensile strength) with comparatively low weight.

Up to the beginning of the 20th century textile materials based either on animal (e.g. wool, silk) or plant fibers (e.g. cotton, hemp). With the rise of synthetic fibers new functionalities are available. Besides traditional textile applications the area of technical textiles was born. A technical textile is a textile product manufactured for non-aesthetic purposes, where function is the primary criterion. Nowadays, technical textiles can be found everywhere and everybody uses such technical textiles although not everybody notices them. Some examples are the conveyor belt at the cash desk in the supermarket, the safety belt, the tire cords and the airbags in cars or the roofs of modern sport arenas. Further applications can be found in medicine (e.g., implant materials, wound dressing), building trade (fiber-reinforced concrete), protective clothing (e.g., bullet-proof vests, heat protection, flame retardance), geo- and agrotextiles (reinforcement of slopes, erosion and crop protection). The sector of technical textiles is large and grows rapidly with a rate of 4 % per year. Nowadays the most widely technical textile materials are used in filter clothing, furniture, hygiene medicals and construction material.

Here, we report our latest approaches on new, innovative technical textiles, e.g., textiles as carrier material for immobilized catalysts, polyelectroyte-functionalized textiles for the recovery of noble metals from industrial waste waters or the decontamination of chromate-polluted soils and new conductive textiles based on conductive polymers and its application as textile-based heating elements.

OM4

Triangulenium Salts. Synthesis, optical properties and self-assembly of cationic π-systems.

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Triangulenium salts (Figure 1a) are rigid planar carbenium ions of exceptional chemical stability, and broad structural diversity.[1] The key steps in the synthesis of various triangulenium ions are all based on efficient and selective nucleophilic aromatic substitution reactions driven by the cationic nature of the precursors and products.[2] After an introduction to the synthesis of the triangulenium salts the talk will focus on two topics: 1) Aza/oxa triangulenium dyes (ADOTA+ and DAOTA+) with long fluorescence lifetimes ($\tau \approx 20$ ns) and their use in bioimaging and detection of protein-protein interactions.[3] 2) Self-assembly of amphiphilic derivatives of amino-trioxatriangulenium salts (ATOTA+). In Langmuir and Langmuir-Blodgett films as well as in bulk the ATOTA+ salts form closely packed columnar aggregates with a strong tendency to form bilayers.[4] However, by changing the associated counterions it is possible to tune the amphiphilic properties of these aggregates and thus modify the aggregate superstructures. The interaction between bilayers of the cationic discotics can be tuned from attractive to repulsive by choice of anion, leading to either multilayer nanorods (Figure 1b) or to monodisperse single-walled nanotubes (Figure 1c).[5]

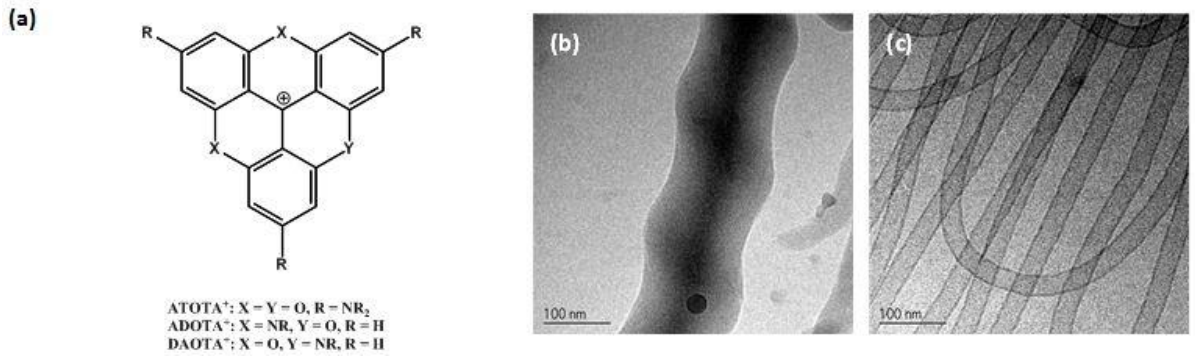

Figure 1. (a) Molecular structures. Cryo-TEM of aggregates formed in aqueous solutions: (b) multi-layer nanorods (c) mono-disperse single walled nanotubes formed by amphiphilic ATOTA+ salts.

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OM5

Endogenous-Inspired Hydrophobic Drug Delivery to Cancers: LDL-like Nano Particles Designed to "Put the Drug in the Cancer's Food"

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This presentation will discuss our new approaches to nanoparticle therapeutic drug and imaging agent delivery, as especially applied to hydrophobic drugs for metastatic cancer. We started by asking, "How did nature solve its own delivery of hydrophobic "drugs" problem?" --the answer being, "With Lipoprotein particles". We are therefore reverse-engineering the LDL as inspiration for anti-cancer drug delivery. Motivation for this approach includes the fact that rapidly growing cancer cells have high numbers of LDLRs, (4-100x greater than on normal cells); numerous malignancies over-express LDLR (brain, colon, prostate, adrenal, breast, lung, leukemias, and kidney); and in patients with cancer, their Low Density Lipoprotein (LDL) count is even known to go down. Furthermore, an abundance of LDLR is a prognostic indicator of metastatic potential, and a propensity to store cholesteryl ester is a sign of the aggressiveness of a patient's cancer. Our choice of drugs focuses on pathway-specific growth and metabolic targets in cancer, that are themselves quite hydrophobic, such as: Tyrosine Kinase of the growth factor receptor – (Lapatinib), Wnt pathway (Niclosamide), Fatty acid synthase (Orlistat), and a variety of Androgen Receptor inhibitors. Thus, if we could reverse engineer the LDL, could it inspire a new pure-drug, ligand-targeted, PET-imageable, nanoparticle, especially for metastatic disease? "Can we put

the drug and the imaging agent in the cancer's food?" "Can endogenous uptake mechanism be used to make cancer cells take up a drug or imageable nanoparticle as though it was an LDL of essential materials --cholesterol, phospholipids, and cholesteryl ester?" But instead of being nutrients that feed the cell, Pure-Drug Nanoparticle (PDN) would retard the cells growth, kill it out right, or cause it to kill itself.

We will report on the progress we have made towards these goals. This includes: 1) Developing further a new method [1] for making nanoparticles by rapid solvent injection, exploring physical and chemical parameters of solvents, test-materials, PET imaging agents and drugs; Characterization of LDL receptor (LDLR) expression level in human mammary epithelial cell lines, involving techniques such as, Quantitative Polymerase Chain Reaction, Western Blot, Flow cytometry, Isogenic cell line technology and Live Cell Imaging; 3) Evaluation of cell cytotoxicity of formulated peptide-targeted drug nanoparticles; and 4) the use of the micropipet technique to explore and inform the nanoscale by observation of solvent injection of miscible and immiscible solvent-solutions, measurements of interfacial tensions, and quantifying micro-droplet dissolution rates leading to dug micro-crystallization or -amorphous formation. All this is building towards an approach to personalized medicine from the theranostic side, utilizing PET-imagable metabolic indicators, EPR evaluation, and pure-drug nanoparticle delivery.

Acknowledgements

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UM - Uorganisk kjemi og materialvitenskap

UM1

COATINGS FOR ANTI-ICING APPLICATIONS

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Ice accumulation on ships, offshore constructions and telecommunication equipment is a challenge when exposed to weather conditions where ice can be formed. Currently, electrical heaters, hot air sources and addition of chemicals (e.g salt and glycols), are the most used anti-icing or de-icing techniques. However, these techniques are not optimal. As alternative, passive techniques such as material choices, structural surfaces and coatings have received increased attention.

Hydrophobic anti-icing coatings, that successfully repel water and prevent ice accumulation, are of great importance. This will greatly enhance operational efficiency, life-time, and safety of constructions and materials exposed to harsh environment in cold-climate regions.

In order to increase the hydrophobicity and anti-icing performance of a coating, a low surface energy (low degree of wetting) and a characteristic topology of the exposed surface are of particular interest.

Here we present a study on silane-coatings for anti-icing purposes. Different silane precursors were used as starting materials due to different hydrophobic groups. Through a hybrid inorganic-organic sol-gel synthesis, the coatings were prepared, and coated on Si-wafers of different surface topography. Areas of importance are:

- The effect of type of fluorosilane precursor
- The effect of different sol synthesis parameters
- Different coating deposition methods
- The impact of surface morphology
- The effect of thicker coatings (several layers)

The sols were investigated by NMR, FT-IR, viscosity and pH. The coatings were studied by using contact angle measurements, AFM, SEM/EDS, profilometer and white light interferometry, and icing properties of the coatings were finally studied.

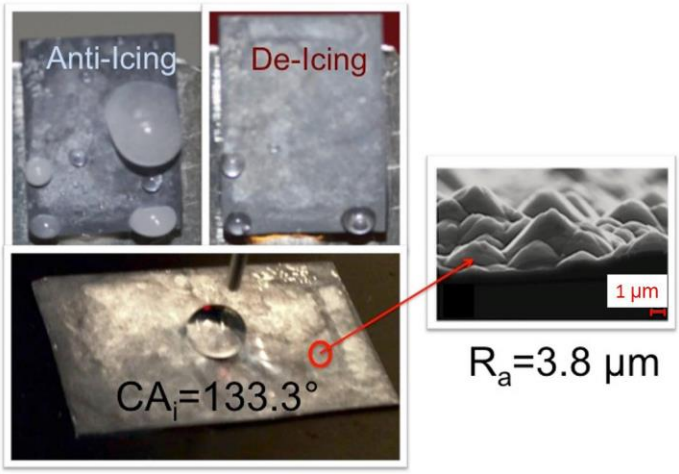

Fig. 1: A coated Si-substrate with high water contact angle and its microstructure.

UM2

HYPER-EXPANDED FeSe-BASED SUPERCONDUCTORS

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The discovery of superconductivity at critical temperatures, Tc, as high as 48 K in iron selenide based materials with formula M_xFe_2-ySe_2 (M = K, Rb, Cs and Tl) has generated considerable excitement [1-5]. High-temperature solid-state synthesis leads to highly defective and inhomogeneous samples. Instead, low temperature reaction of FeSe with a solution of alkali metal in liquid ammonia is a viable route to obtain single-phase materials. Indeed, ammonothermal synthesis has been employed and different phases with nominal composition $M_xFe_2Se_2$ (M = Li, Na, Ba, Sr, Ca, Yb and Eu) were isolated [2]. Intercalation results in a drastic increase of the interlayer spacing, and the superconducting temperature reaches 46 K in $(NH_3)_x$Li@FeSe [3]. Here we report a detailed in situ PXRD (SNBL/BM01B beam-line at the ESRF) and SQUID magnetometry (UiO) study of the reaction between Ba and FeSe in liquid ammonia solutions; crystal structures and magnetic properties of final and intermediate phases were investigated to understand the influence of the interlayer spacing on the properties of the superconducting and normal state. At least 6 various Ba@FeSe phases were observed as metastable and stable intermediates between FeSe and stable ammonia-free Ba@FeSe with critical temperature Tc = 36 K. Intermediate phases show variations in interlayer distances (d = 13.14 – 8.38 Å, see Figure) and as a result various superconducting temperatures (Tc = 39 – 34 K) [4-5]. In particular phase I and phase II show the largest interlayer spacing ever reported. Reaction FeSe + Ba → Phase I has $\tau_{1/2}$ ~ 2-3 min and subsequential reaction Phase I → Phase II is relatively slow ($\tau_{1/2}$ ~ 70 min). Importantly, phases I and II show the largest interlayer spacing ever reported in any analogous system but not the highest Tc. This observation contradicts the common understanding of the properties of these materials and opens a number of questions on the real influence of the interlayer distance on the superconducting mechanism.

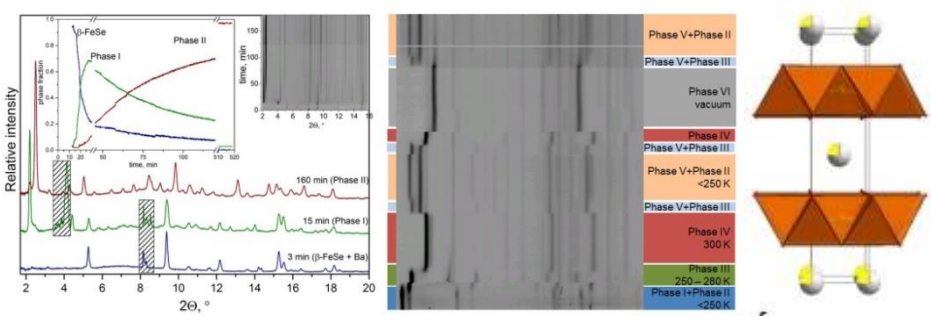

Figure. *Left*: PXRD data (λ = 0.504850 Å) obtained for Ba and β-FeSe mixture at 200 K (diffraction lines characteristic for Ba and $BaNH_x$ phases are striked out). Insets show time dependence of diffracted intensity and phase fraction for β-FeSe, Phase I and Phase II obtained from Rietveld refinement. *Middle*: PXRD data for Ba + β-FeSe after completion of transformation to Phase I. *Right*: crystal structure of Ba@FeSe (phase VI).

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UM3

DEVELOPMENT OF NOVEL BIODEGRADABLE HYBRID NANOPARTICLES FOR CANCER DIAGNOSIS AND THERAPY

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Nanoparticles (NPs) developed from polyhedral oligomeric silsesquioxane (POSS) structures open new perspective in the field of drug delivery. Due to their nanocaged structure consisting of an inner inorganic framewrok of silicon and oxygen atoms, and an outer shell of organic functional groups, these NPs have a unique biomedical application. By the implication of organic chemistry and polymer science different types of POSS based NPs can be obtained.

Nanomicelles can be formed by creating an amphiphilic POSS structure, a POSS structure partially modified with organic fatty acid and long PEG chain. Formation of nanomicelles can facilitate the drug loading of hydrophobic drugs. This will enhance the bioavailability of these drugs.

In the actual work polyhedral oligomeric silsesquoixane POSS structure was modified with behenic acid and PEG methacrylate chains. Different ratios have been used in order to prepare these NP's. POSS based structure is expected to form nanomicelles in the aqueous solution and be stable during long period of time. The results obtained from particle size measurement show that POSS based nanomicelles form agglomerates after dialysis while the average size of 100nm was obtained before dialysis (having organic solvent inside the sample). Preliminary study of hydrophobic drug loading was tested using NR668 a hydrophobic dye Nile Red. Stability of nanomicelles in cell medium was as well investigated.

UM4

Engineering the morphology, composition and structure of PtRh Nanoparticles by Microwave Irradiation Synthesis

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PtRh bimetallic Nanoparticles (NPs) capped with polyvinyl pyrrolidone (PVP) were synthetized by Microwave Irradiation (MIW) dielectric heating. We were able to tune the morphology of the NPs acquiring octopod-cubes, cubes, truncated cubes and small spheres by increasing the molar ratio of PVP to Pt- and Rh precursors, keeping the microwave irradiation time constant (5min). The NPs were characterized by High Resolution Transmission Electron Microscopy (HRTEM), Energy Dispersive X-ray Spectroscopy (HRTEM-EDS), X-Ray diffraction (XRD) and X-ray Photoelectron Spectroscopy (XPS). TEM analysis revealed near monodispersed NP distributions, covering the range from 3 to 18 nm. XRD, XPS and EDS results show that the produced NPs consist mainly of Pt, while Rh is detected only for the lowest PVP concentration. XPS measurements indicate that the surface is enriched in Rh, indicating a core shell structure. The composition of the PtRh NPs was tuned by changing the time parameter of the MIW synthesis. Increasing the total MIW time up to 20 min we were able to prepare alloy $Pt_{100-x}Rh_x$ NPs with $x < 50$, while keeping equimolar precursor's concentration, see Fig. 1. Incorporation of Rh in the alloying process make it complicated to control shape and the size of the NPs.

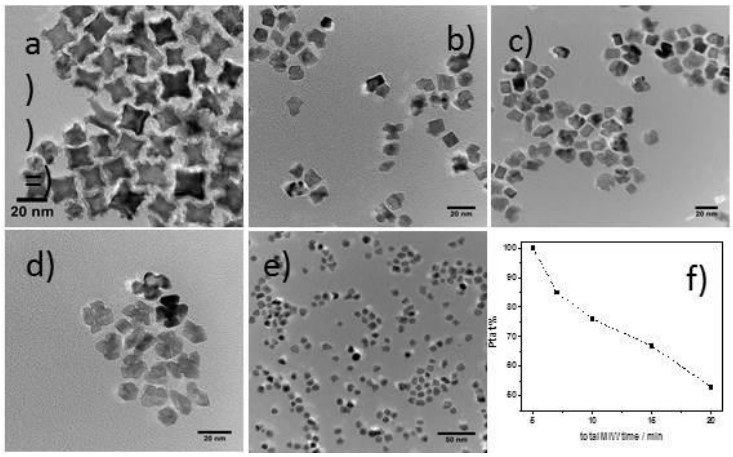

Fig. 1: HRTEM images of PtRh NPs prepared at a)5min, b) 7min, c) 10min, d)15min and e) 20min of microwave irradiation. Graph f) shows the at.% of Pt calculated from the EDS spectra.

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UM5

A MASTER MODEL FOR PROTON CONDUCTING MATERIALS

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Proton conduction is observed in materials over temperatures ranging from ambient to above 1000°C, and applications comprise as different materials as the polymer proton exchange membranes (PEMs) operating below 100°C, the solid acids like CsH_2PO_4 operating around 200°C, and proton conducting oxides, operating typically at 600°C. The discoveries of new families of proton conductors are claimed, such as high-temperature N-containing polymers like poly-benzimidazole, pyrophosphates like SnP_2O_7, and nanograined or nanoporous ceramics of otherwise oxide ion conducting YSZ and GDC. Most of the proton conductors exhibit a maximum in conductivity with increasing temperature, reflecting the combined action of increasing mobility of protons or protonated species on the one hand, and decreasing concentration through dehydration. There has nevertheless been little general recognition of common features, and moreover, there are conflicting reports of phase purity, proton conductivity, and interpretation and mechanisms involved.

In this contribution, we present for the first time a more global view - a kind of a master model and a generic master Arrhenius-type temperature dependency - of the protonic conductivity contributions that a typical materials sample may have. For an acceptor-doped oxide ceramic, this involves conduction of free protons, peaking at typically a few hundred degrees centigrade, and protonic conduction in the ad- and absorbed water in open grain boundary cores and porosity. The latter comprises conduction in single and multiple layers of adsorbed water - increasing with decreasing temperature - and in condensed water, increasing strongly towards the dew point in the surrounding atmosphere. Both carrier concentration and hydration can be affected by "doping" the material and hence internal surfaces with oxyacid groups.

As temperature is lowered further the condensed water exhibits a maximum in conductivity and decreases with decreasing mobility. Freezing may add to this.

All in all, the temperature dependency of the protonic conductivity of a ceramic oxide exhibits two maxima at high and ambient temperatures, respectively, and the latter has many features in common with the conductivity of proton exchange polymers membranes (PEMs) and acid-doped pyrophosphates, and we will discuss this in terms of a uniform model.

Acknowledegement

Work supported by the Research Council of Norway, RENERGI "NaProCs" 216039.

UM6

DEFECT CHEMISTRY OF HEXAGONAL MANGANITES FROM FIRST PRINCIPLES

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Hexagonal manganites have attracted considerable attention due to their multiferroic properties [1, 2], but has also recently shown promise for energy technology purposes. Due to their layered crystal structure, the hexagonal manganites can accommodate interstitial oxygen, which are not common in perovskites. Hexagonal $Dy_{1-x}Y_xMnO_{3+\delta}$ can accommodate excess oxygen up to $\delta < 0.35$ at relatively low temperatures of 250-400 ºC [3], opening the possibility for use as oxygen storage materials at much lower temperatures than the present state-of-the-art materials [4, 5]. Oxidation of the multivalent manganese ions could be the charge compensating mechanism, creating holes in the valence band of $YMnO_3$ and p-type semiconductivity. [6].

Hexagonal manganites can also be oxygen deficient, and show strongly anisotropic chemical expansion. Flexoelectricity in hexagonal manganite thin films has been attributed to oxygen vacancies creating stress fields due to the chemical expansion. [7, 8]. Computational studies on chemical expansion will become increasingly important as transition metals oxides are integrated into electronic circuitry. [9].

A-site deficiency will also be addressed as our preliminary studies have demonstrated that YMnO3 can accommodate up to 30 % Y deficiency with surprisingly small structural changes.

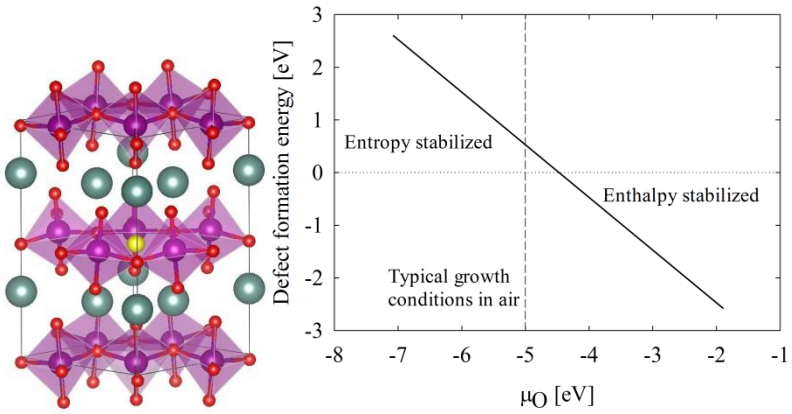

Fig. 1: a) Interstitial oxygen in most stable position in $YMnO_3$. b) Defect formation energy for interstitial oxygen as a function of chemical potential of oxygen in $YMnO_3$.

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UM7

HYDRATION AND INTERCALATION IN RUDDLESDEN-POPPER PHASES

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Ruddlesden-Popper (RP) type oxides, $A_{n+1}B_nO_{3n+1}$, possess a wide range of technologically important properties; i.e. thermoelectricity, colossal magneto-resistance, mixed conductivity and high temperature superconductivity. RP oxides are also currently of high interest in solid oxide fuel cell (SOFC) technology. The RP structure consists of n blocks of perovskite type units (ABO_3) separated by a layer of rock salt type (AO). Certain $A_4B_3O_{10}$ (n=3, RP3) materials are prone to intercalation reactions with water, carbonate and simple alcohols after treatment in reducing atmospheres [1, 2]. Several show major oxygen intercalation. The intercalated species locate to the rock salt layers, however, the process and the accompanying structural and physical changes are poorly understood. Their electric transport properties are

affected by intercalation, such as changing from mixed to ionic conduction. The properties can be modified by careful tuning of the oxygen stoichiometry and type and concentration of the intercalating species. In addition to the focus on intercalation, we explore novel solid solution systems with intriguing physical properties, including redox activity and vacancy ordered superstructures. The goal of this presentation is to demonstrate the interplay between the structural, electronic and magnetic properties of RP3 phases as a function of intercalation.

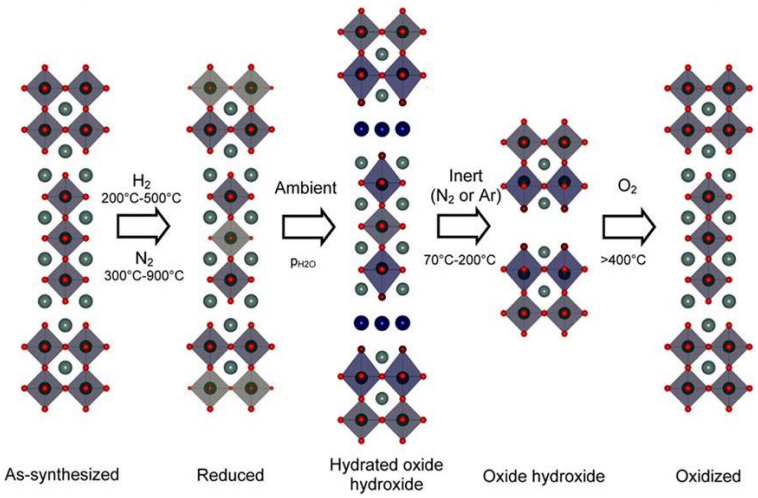

Fig. 1: Structural change throughout water intercalation and de-intercalation process

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UM8

REVISITING RHOMBOHEDRAL LEAD METANIOBATE: CRYSTAL STRUCTURE AND FUNCTIONAL PROPERTIES

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Lead metaniobate ($PbNb_2O_6$) can exist both as a stable rhombohedral and a metastable orthorhombic tungsten-bronze-type polymorph.[1,2] Although the tungsten-bronze is a well-known ferroelectric material, the rhombohedral polymorph (Fig. 1) has been far less studied. The crystal structure and energetic stability of the stable rhombohedral polymorph of lead metaniobate is re-examined by powder X-ray diffraction and powder neutron diffraction, in

combination with ab initio calculations.[3] We show that the structure is described by the polar space group R3, in contradiction to the previously reported space group R3m. The polar space group opens up for possible device applications of the material, and investigations of the high-temperature behaviour of the materials also hint towards interesting functional properties.

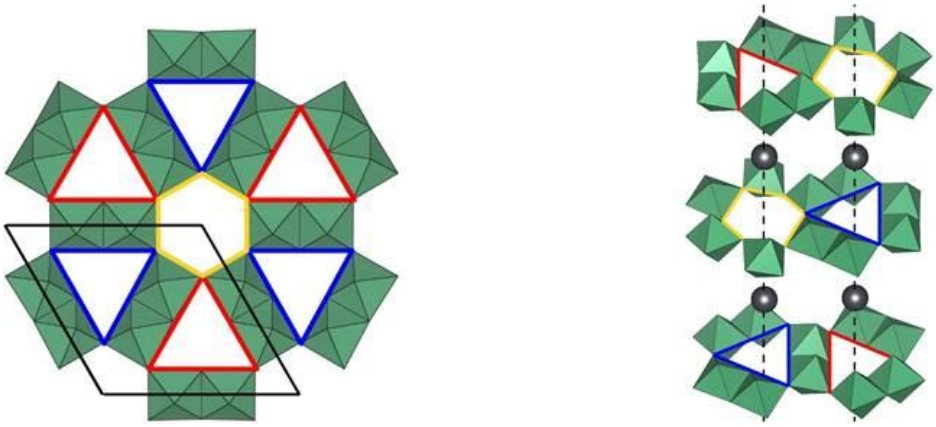

Fig. 1: The crystal structure of rhombohedral lead metaniobate. Left: Single layer built from Nb_2O_{10} dimers; Right: Stacking sequence of layers with Pb^{2+} in channels along [001].

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UM9

CRYSTAL CHEMISTRY AND THERMAL PROPERTIES OF RARE EARTH BOROHYDRIDES

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Rare earth (RE) borohydrides have received considerable attention during the past 5 years due to their rich crystal chemistry [1-4] and potential as both solid state hydrogen storage materials and solid state electrolytes [5]. Mechanochemical synthesis that utilizes a metathesis reaction between a RE-chloride and an alkali metal borohydride (mostly $LiBH_4$) is now the standard technique for the synthesis of RE-borohydrides. RE-borohydrides form distinct structure types which are determined by the ionic radius of the RE and its electronic configuration. The early lanthanides La, Ce, Pr, and Nd form $LiRE(BH_4)_3Cl$ compounds (cubic; I-43m), where each RE is octahedrally coordinated by three BH4- units and three Cl atoms, while the RE and Cl atoms in the unit cell form a distorted Re_4-Cl_4 cube. Sm, Gd, Tb, Er and Yb form α-$RE(BH_4)_3$ (cubic; Pa-3) with a possible polymorphic transition to β-$RE(BH_4)_3$ for Y, Yb (cubic; Pm-3m or Fm-3m). α/β-$RE(BH_4)_3$ borohydrides are related to the ReO_3-structure type where the RE atoms are situated at the corners of a cube and the BH_4

units lie along the edges leading to an octahedral coordination of RE by six BH_4 units. The smallest lanthanides Yb and Lu form tetrahedral $[RE(BH_4)_4]$- anionic complexes that are stabilized by Li+ cations (tetragonal; P-42c) in analogy to $LiSc(BH_4)_4$. Furthermore, Sm and Gd show transitions to the $LiRE(BH_4)_3Cl$ structure type that is observed for the largest lanthanide ions [2, 3].

Composite mixtures between a RE-borohydride and $LiBH_4$ are interesting for hydrogen storage purposes because excess $LiBH_4$ can be destabilized via the formation of RE-hydrides which results in significantly reduced desorption temperatures [3]. We have investigated a wide range of composites based on $6LiBH_4$-$RECl_3$-3LiH and present experimental results based on in/ex-situ powder X-ray diffraction, thermogravimetric and caloric measurements, and cycling experiments for La- and Er-based borohydrides.

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UM10

STRUCTURAL AND MAGNETIC ASPECTS OF $La_4(Co_{1-x}Ni_x)3O_{10+\delta}$ (0=< x =<1)

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$La_4(Co_{1-x}Nix)_3O_{10+\delta}$ bridges two Ruddlesden-Popper RP = 3 phases with quite different properties: Pauli-paramagnetic $La_4Ni_3O_{10+\delta}$ with metallic like conductivity [1] and the antiferromagnetic $La_4Co_3O_{10+\delta}$ semiconductor [2]. $La_4Ni_3O_{10+\delta}$ is reported as orthorhombic [1] whereas $La_4Co_3O_{10+\delta}$ is monoclinic [2, 3]. However, a broadening of (117) in the X-ray diffractograms suggests monoclinic distortions also for $La_4Ni_3O_{10+\delta}$. A number of structural deformations (and space groups) as function of composition (x) are proposed by Amow et al. for $La_4(Co_{1-x}Ni_x)3O_{10+\delta}$ [4].

The current neutron diffraction analysis indicates no structural change when going from $La_4Co_3O_{10+\delta}$ to $La_4Ni_3O_{10+\delta}$. For all compositions it is feasible to adjust the oxygen content (δ) by annealing at fixed temperatures by varying oxygen partial pressure, tuning the amount of trivalent Co- and Ni-cations. Oxygen analysis is done by cerimetry and TGA. The magnetic

and electric properties are strongly composition dependent (x, δ). Finally, the results from the various measurements is summarised in a phase diagram of structural and electronic properties of the complete solid solution $La_4(Co_{1-x}Ni_x)3O_{10+\delta}$.

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UM11

ZEG Power - more energy and less emissions

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The ZEG-technology (Zero Emission Gas - **ZEG®**) is a hybrid technology for co-production of electricity and hydrogen from hydrocarbon fuels, with integrated CO2-capture. The main strengths of **ZEG®** for energy production are high overall efficiency, in the range of 70 to more than 80% depending on the plant size, and the flexibility; all types of carbon based fuels can be used, product composition can be varied dependent on market demand and applications and scale are from small scale distributed plants based on biogas to industrial scale gas power plants.

The basic technologies in the ZEG-concept are electricity production by SOFC (solid oxide fuel cells) and hydrogen production by a modified steam reforming reaction, (SER - sorption enhanced reforming). Close thermal integration of the two basic technologies is necessary in order to obtain a high total efficiency.

The technology will be presented included main results from the basic technologies, status and plans for further technology development.

UM12

Steam to hydrogen using high temperature proton ceramic electrolyser cells

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Renewable energy sources are gradually becoming more important to the largest energy markets worldwide, as fossil fuel and nuclear power plants are phased out. As the market share of intermittent energy sources such as wind and solar continue to grow, it is of vital importance to develop cost efficient and clean energy storage technologies to store peak hour energy. High temperature electrolysis (HTE) of steam offers high efficiency of conversion of renewable and peak electricity to H_2 and may increase efficiency further by utilising available sources of heat and steam from solar, geothermal, or nuclear power plants. Technologies developed to date comprise solid oxide electrolyser cells (SOECs) utilising oxide ion conducting electrolytes operating by virtue of necessity around 800 °C. They produce hydrogen on the steam feed side, and separation and drying of H_2 costs energy and add plant complexity and footprint. In comparison, a high temperature proton conducting electrolyte will instead pump protons (H+) and form dry H_2, leaving O_2 on the steam side. Such proton ceramic electrolyser cells (PCECs) thus require less separation process stages and can produce pressurised dry H2 directly. Protons exhibit lower activation energies than oxide ions, and ceramic proton conductors should be able to operate at lower temperatures – 600-800°C – i.e., closer to the ideal range for integration with solar and geothermal plants.

This contribution will outline the general concepts of steam electrolysis with emphasis on the different electrochemical processes that occur throughout the electrolysis cell, and the remaining material challenges that must be resolved for proton ceramic electrolyser cells to be competitive as a cost efficient energy storage technology: i) Development of novel H_2O-O_2 anodes comprised of composite oxide materials that display mixed proton-electron conductivity, high catalytic activity towards water splitting, and compatibility with the electrolyte material; ii) development of scalable fabrication routes for complete electrolysis cells that can withstand 50 bar steam at 600-800°C for long durations.

UM13

STRIKING HYDROGEN UPTAKE BEHAVIOR DIFFERENCES IN CPO-27 MATERIALS INDUCED BY METAL SUBSTITUTION

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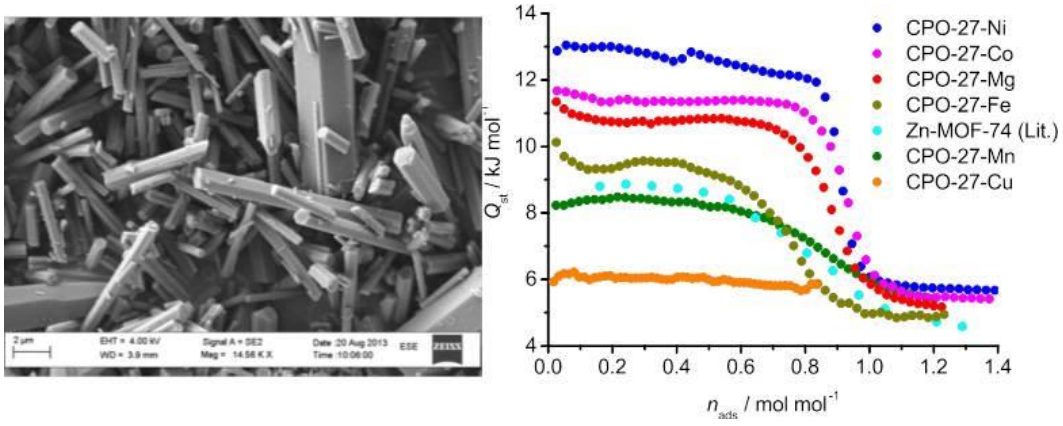
Metal-organic framework materials have shown remarkable hydrogen uptake and sorption properties. Among the most intriguing series of compounds are the isostructural microporous coordination polymers [M_2(dhtp)] (CPO-27-M, M-MOF-74 or M_2(dobdc)), in which a high concentration of coordinatively unsaturated metal sites results in high initial heats of adsorption.[1]

We present a comparative study of hydrogen gas adsorption experiments on CPO-27-Cu and -Mn, which show striking differences in their hydrogen uptake behaviors which can be attributed to the difference in interaction between hydrogen and the respective metal cation incorporated in the framework structure. Inelastic neutron scattering experiments were carried out to confirm the remarkable difference and gain further insight into the adsorption process. Firstly, CPO-27-Cu demonstrates the lowest isosteric heat of adsorption for H2 of all the CPO-27-M materials reported to date, where M = Ni, Co, Mg, Zn, Mn, and Fe,[1] and CPO-27-Mn the second lowest. Secondly, all the reported CPO-27 materials show two steps in the adsorption isotherm and two distinct values corresponding to the first and second adsorption sites in the heats of adsorption, which are not observed for the CPO-27-Cu. Thus, the open metal site and second adsorption site are energetically equivalent in CPO-27-Cu, and there is no preference for the hydrogen gas at the open metal center.



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UM14

SODIUM- AND POTASSIUM CONTAINING THIN FILMS BY ATOMIC LAYER DEPOSITION

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Sodium- and potassium containing complex oxides exhibit a range of properties important for applications in present and future materials technology. Examples of such compounds include ferroelectric $K_xNa_{1-x}NbO_3$ [1], the battery cathode material Na_xMnO_2[2] and thermoelectric Na_xCoO_2[3], finding their use on devices such as sensors, actuators and devices with need for integrated energy supply. As devices become smaller, the need for techniques enabling deposition of thin films with sub-nanometer thickness control and high conformality becomes increasingly important. Atomic layer deposition is a well-established technique that accommodates these criteria[4]. Processes for depositing oxides of most common elements have already been reported[5], with exceptions including many of the important alkali metals

due to lack of suitable precursors. In this research, we highlight some crucial challenges of atomic layer deposition of compounds containing sodium and potassium and how these can be overcome, including presentation of suitable precursors. Deposition of some technologically interesting materials is used to support the impact this progress may have for future thin film research.

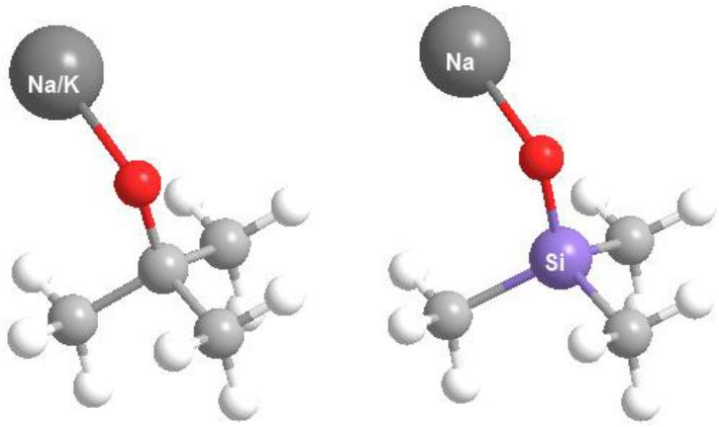

Fig. 1: The two precursors enabling atomic layer deposition of sodium- and potassium containing thin films.

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UM15

LUMINESCENT LANTHANIDE TITANATES BY ALD

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LUMINESCENT LANTHANIDE TITANATES AND LANTHANIDE YTTERBIUM TITANATES HAVE BEEN GROWN BY ALD FOR LIGHT CONVERSION

Lanthanide oxides is an important class of functional materials, used as light converters in phosphor materials, active media in lasers, fuel cells and magnetic materials to name a few. Atomic layer deposition (ALD) gives unique possibilities in tailoring doping profiles and compositions not easily reproduced by other methods. Controlling the film growth and growth parameters of the lanthanide oxides thus enables novel structures and materials to be synthesized.

Based on our previous work on ALD films of Ln_2O_3[1], $Eu_xTi_yO_z$[2] and nanolaminates of Eu_2O_3/TiO_2 sandwich structures[3], we here explored the luminescent properties of $Ln_xTi_yO_z$

and $(Ln,Yb)_xTi_yO_z$ film materials. The goal is to achieve efficient UV-to-NIR light conversion through UV absorption in TiO_2 and 1000 nm emission of Yb^{3+}, with or without and intermediate step through a second lanthanide Ln^{3+}.

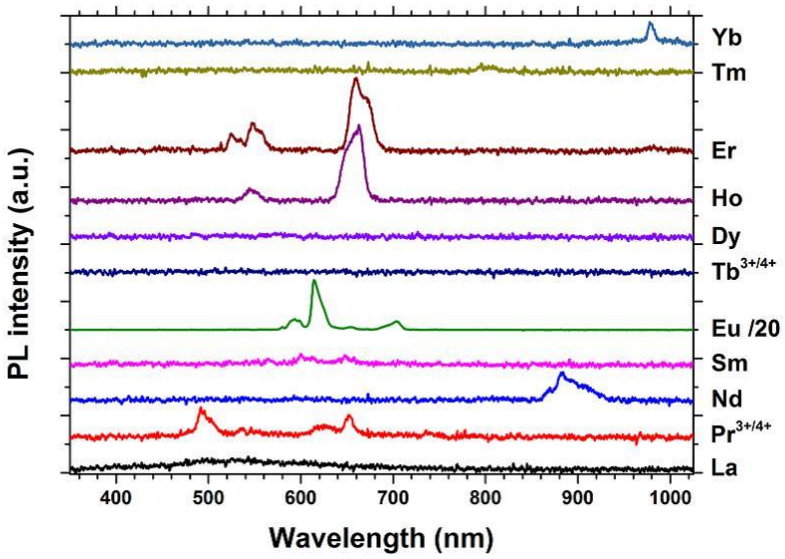

Fig. 1: Visible and NIR emission of $Ln_xTi_yO_z$ thin films, excited by 325 nm HeCd laser.

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UM16

Ferroelastic hardening in ferroelectric $(1-x)Bi_{0.5}K_{0.5}TiO_3$–$xBiFeO_3$ (x = 0.8, 0.9)

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Lead-free piezoelectric materials have gained significant attention in recent years[1]. One of the highly interesting materials is $BiFeO_3$ (BFO) with a high strain and polarization, and possible high temperature applications due to the high TC. The application of BFO is though challenging because of a high coercive electric field and a problematic electrical conductivity [2]. Due to the synthesis challenges of pure BFO, $(1-x)Bi_{0.5}K_{0.5}TiO_3$ –$xBiFeO_3$ ((1-x)BKT - xBFO, x = 0.8, 0.9)has been studied as a model system to better understand the point defect chemistry and electrical conductivity of BFO[3].

The high coercive electric field of BFO has been related to point defects that arise due to evaporation of Bi_2O_3during fabrication [4]. Point defects due to this loss may act as pinning centers for domain walls and hamper wall movement, reducing the polarization and strain observed for polycrystalline BFO. The hard ferroelectric properties of BFO have motivated the present study of ferroelastic properties, possibly related to the same phenomenology. An advantage of ferroelasticity is that challenges related to conductivity and dielectric breakdown at high electric field are avoided.

Here we report on a study of aging/hardening in relation to point defects in BKT-BFO by stress-strain measurements in samples with different thermal history and with donor doping. Sintered samples were grinded to a cylinder shape and annealed above TC to relieve residual stresses. A uniaxial stress up to 800MPa was applied on the samples at temperatures up to 400°C. Crystal structure and phase transitions were examined by high temperature X-ray diffraction, thermal analysis and dielectric spectroscopy.

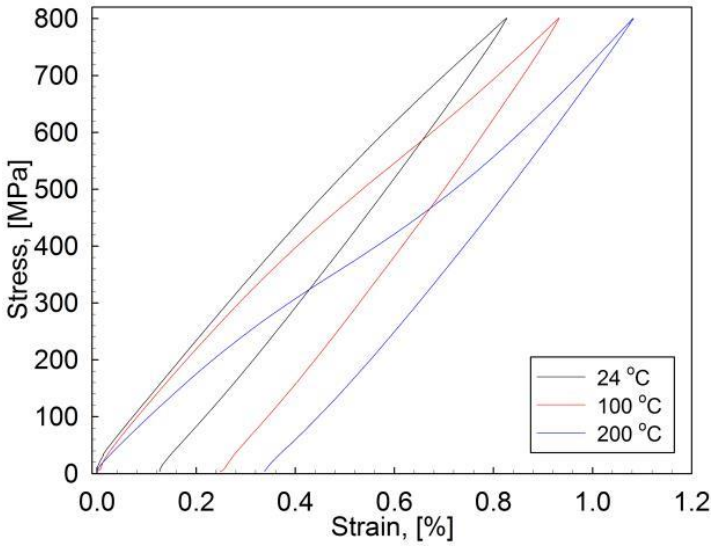

Fig. 1: Temperature dependence of stress-strain curves for 0.8BFO.

The results show that the thermal history of the materials is of great importance for the stress-strain curve. A furnace cooled sample (300°C/h) i.e. shows no ferroelastic behavior while an air quenched sample demonstrates opening of the stress-strain curve and remanent strain. The ferroelastic properties were found to vary significantly with temperature (Fig. 1). It was also found that the crystal structure and the ferroelastic properties were sensitive to donor doping which further implies that the point defect chemistry of the material is of great importance.

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UM17

STABILITY OF CARBON CONDUCTIVE ADDITIVES AT HIGH OPERATING VOLTAGES IN LI-ION CATHODES

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Carbon conductive additives are important constituents of the Li-ion battery cathodes, as the oxidic cathode materials used up to now are suffering from too low electronic conductivities. The next generation, high capacity cathodes are expected to operate at higher voltages than the current state-of-the-art cathodes, which will be challenging for the stability of the carbon conductive additive. It is already know that the anion PF6- intercalates in graphite at potentials above 4.2 V, and also that decomposition of electrolyte and exfoliation of graphite due to co-intercalation of electrolyte may occur [1,2]. At higher voltages all know electrolytes will oxidize, which in particular cause degradation of high surface area conductive additives, like carbon black.

The purpose of this study is to compare different carbon conductive additives with respect to their electrochemical performance at high cathodic voltages. In addition to conventional graphite powder KS6 and the carbon black SuperP Li from TIMCAL, a multilayer graphene powder was included in the study. Electrodes from these materials were then cycled galvanostatically in coin cells at various rates, and investigated in 3-electrode experiments with cyclic voltammetry and impedance spectroscopy. The electrolytes used were 1M $LiPF_6$ in 3:7 EC:DMC or 1:1 EC:DMC.

Results show that the intercalation potential of PF_6- is slightly higher for multilayer graphene compared to KS6, and also more reversible. On the other hand, the graphene has a much higher irreversible capacity loss in the first cycle, indicating more severe electrolyte oxidation, although the BET surface areas are similar. All materials showed stable performance upon galvanostatic cycling at 120 mAh/g. Apart from electrolyte oxidation products, no changes to the electrodes could be observed by SEM after cycling. In-situ X-ray spectroscopy was performed to obtain more information on the anion intercalation processes in the multilayer graphene material as compared to the graphite material. The results were relatively similar for the two materials, and show that the intercalation of PF6- is only partly reversible.

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UM18

Investigation of the electrical conductivity in LiAlO2 thin films deposited by Atomic Layer Deposition

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Atomic Layer Deposition (ALD) allows deposition of highly conformal films on complex and 3-dimensional (3D) structures. It has been recognized as a suitable and promising tool to achieve solid-state and 3D designs to obtain safer and more robust Li-ion battery systems. Recent successful deposition of Li-containing thin films by ALD [1-3] opened up new possibilities to develop solid-state electrolytes as well as other active materials for Li-ion (micro)batteries. For the moment, the investigation of potential solid-state electrolytes by ALD is still new [3] and there are currently very few reports on the crucial characteristic – Li-ion conductivity in such thin films [4-6], especially at room temperature. This is probably due to the low Li-ion conductivity in solid state and the challenges in conducting electrical measurement on amorphous thin films.

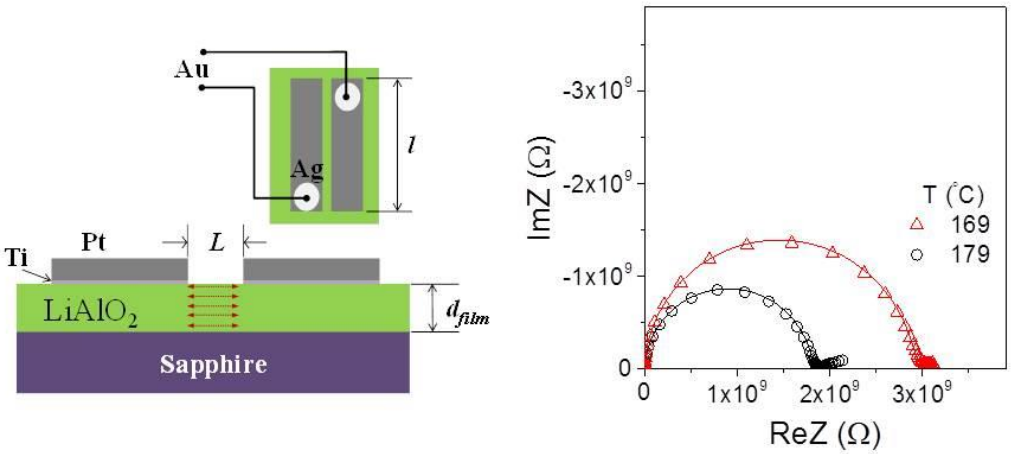

Fig. 1. (a) Geometrical configuration of in-plane conductivity measurement. (b) Impedance spectra of 160 nm-thick LiAlO2 thin films on sapphire substrate obtained by in-plane measurement. The inset shows the equivalent circuit for data fitting, and the solid lines represent the fitting results.

$LiAlO_2$ have been deposited by ALD [5] and were utilized as barrier and protection layers [5,7] in Li-ion batteries. This work aims at investigating the conductivity properties of the ALD $LiAlO_2$ amorphous films in the temperature range of interest. Electrical characterizations were carried out by impedance spectroscopy from ambient to elevated temperature in controlled atmosphere. An optimized "soft" contacting method is used to make effective and stable electrode contacts. We applied both in-plane and cross-plane measurements, depending on the type of substrate. The conductivities obtained using the cross-plane method are relatively independent of the film thickness, whilst results from in-plane measurements exhibit a stronger thickness-dependence. Room-temperature conductivity in these amorphous $LiAlO_2$ films could be readily measured, and the temperature-dependent

ionic conductivity obtained from the two methods are reported and compared. .

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UM19

EFFECTS OF SINTERING ADDITIVES ON $BaZr_{1-X}Y_XO_{3-\delta}$ DENSIFICATION, STABILITY, AND CONDUCTIVITY

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This work reports on the investigation of $BaZr_{0.9}Y_{0.1}O_{3-\delta}$ (BZY10) and $BaZr_{0.9}Y_{0.15}O_{3-\delta}$ (BZY15) materials for application in Proton Conducting Fuel Cells fed with biogas. Materials were synthesized by Pechini route or solid state reactive sintering with Ni, Mg, Mn, Cu, or Zn as sintering additive. Sintering mechanisms for both routes were studied by in situ optical dilatometry analysis in controlled atmosphere, thermogravimetric and differential thermal analysis, high temperature scanning electron microscopy, in situ X-ray diffraction, transmission electron microscopy and DFT calculations. This study enabled to identify the effects of additive types and content as well as temperature on the densification rate and structure of BZY materials.

Dense samples were successfully produced when using Ni and Zn oxides, after sintering in air at 1500 °C and 1375 °C, respectively. BZY samples produced with Cu, Mg, and Mn oxides remain porous up to 1600 °C. Stability of Cu-, Ni-, and Zn-containing BZY materials in biogas conditions was investigated by thermogravimetric analysis in mixtures of 60% H_2, 10% H_2O, 10% CO_2, 20% Ar, and 800 ppm H_2S. While Ni-BZY samples remain stable under these conditions, both Zn and Cu-doped BZY samples experienced significant changes, attributed to evaporation and sulphidation, respectively, of the dopants.

The conductivity of BZY15 was studied by impedance spectroscopy as function of atmosphere, processing routes and additive contents. Samples prepared from both routes exhibited similar bulk conductivity in wet air with an activation energy of ~0.48 eV (Fig 1). In a wet mixture of 5% H2:95 % Ar, the conductivity of the samples prepared by solid state increased an order of magnitude compared to that in air, whereas no change in conductivity was observed in samples prepared by the Pechini route. These results will be discussed in this presentation.

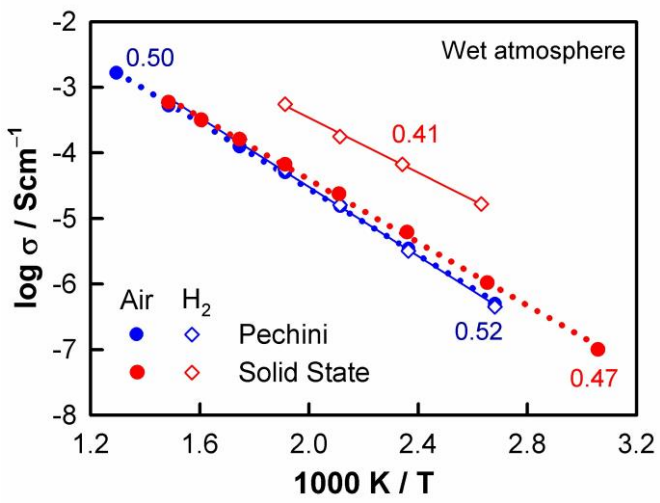

Fig 1. Bulk conductivity Arrhenius plots for BZY15. Numbers represent activation energies.

UM20

ADDITIVES IN MAGNESIUM BOROHYDRIDE: LOCAL STRUCTURE AND EFFECT ON REVERSIBILITY

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Magnesium borohydride is a particularly interesting material for hydrogen storage due to its light weight and 14.9 wt% of hydrogen. Up to about 4 wt% have been found to desorb reversibly below 300^{o}C and at a moderate pressure [1]. For rehydrogenation of the completely dehydrogenated material, however, much harsher conditions are needed [2]. In order to improve hydrogen sorption performance of $Mg(BH_4)_2$, a wide range of approaches are explored, including high energy reactive ball-milling, preparation of composite materials, dispersion in porous matrix, and addition of catalysts [3].

Transition metal compounds have been widely explored for enhancing hydrogen storage properties of complex hydrides, including metal borohydrides [2, 3]. A number of the additives were shown to reduce significantly hydrogen release temperature during the first decomposition of $Mg(BH_4)_2$. However, the effect of additives on hydrogen absorption and further cycling was scarcely studied. In this contribution we present our recent studies on the effect of transition metal–based additives in $Mg(BH_4)_2$. A range of the nickel and cobalt compounds was ball-milled with $Mg(BH_4)_2$, and the sorption properties of the composites were studied upon one or three H-sorption cycles. The desorption and absorption were carried out at 285^{o}C where $Mg(BH_4)_2$ was shown to be reversible at least for one cycle. The additives were characterized by x-ray absorption spectroscopy (XAS), which gives an insight into the local state of metal atoms and the additives composition upon cycling.

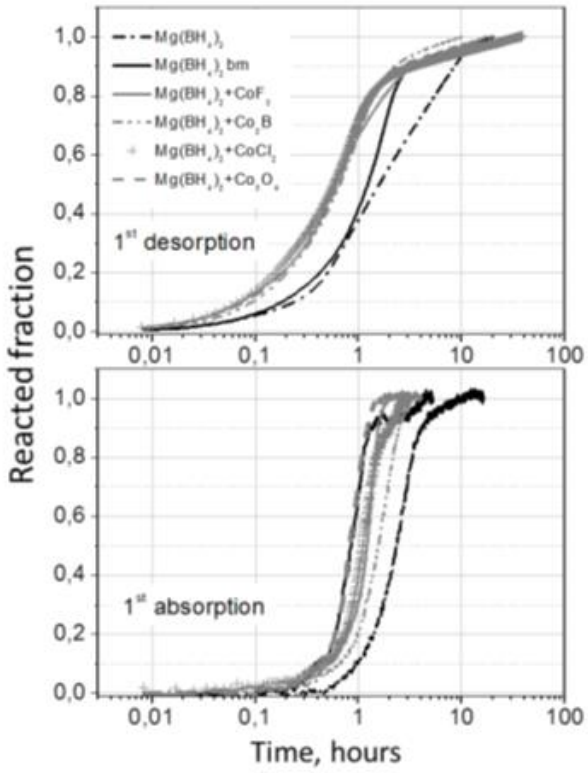

Fig. 1. Desorption and absorption isotherms for $Mg(BH_4)_2$ as such, ball-milled (bm), and ball-milled with additives

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UM21

POWDER SYNTESIS AND PROCESSING FROM NANO TO MILLIMETER SCALE

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Powders, ranging from nano- to millimetre scale, are used for a wide range of applications in the chemical, metallurgical, pharmaceutical and food industries. SINTEF Materials and Chemistry performs work related to development of several technologies where synthesis of powders is essential, e.g. for catalysts, sorbents, batteries, membranes, fuel cells and medical

applications. Tailoring of both chemical compositions and particle morphologies through reproducible and scalable processes is essential for future technology development.

Nanostructured materials are gaining widespread use and require new approaches to synthesis, in particular with respect to increased production while maintaining proper HSE procedures. Flame spray pyrolysis is an excellent tool for pioneering development of complex nanomaterials for various applications, and is also a scalable process already implemented by commercial powder producers. Use of newly invested flame spray pyrolysis unit for synthesis of small scale reproducible batches (1-10 grams) of finely dispersed nanoparticles of various inorganic materials (e.g. mixed oxides) will be presented, along with their potential application areas. Examples of how varying the precursor solution system, liquid- and gas flow rates, as well as gas composition (oxidizing-inert atmosphere) affect the morphology, crystallinity and chemical composition of the product will be given.

For lab scale materials to be attractive for commercialization, viable routes for up-scaled fabrication and shaping at an industrial level need to be developed, while maintaining composition and properties. Spray drying is common route where spherical, dense particles are formed by drying of a droplets formed by atomizing. The particle size typically scale with the size of spray dryer due to increased drying time. Other methods where the final particle size can be easily tailored are granulation, agglomeration and spray coating. The latter methods can scaled up more easily from lab to full scale. All these methods result in different final material properties suitable for a variety of applications. Results from different projects related to processing of powders using the above mentioned techniques will be presented – two examples given in Fig. 1.

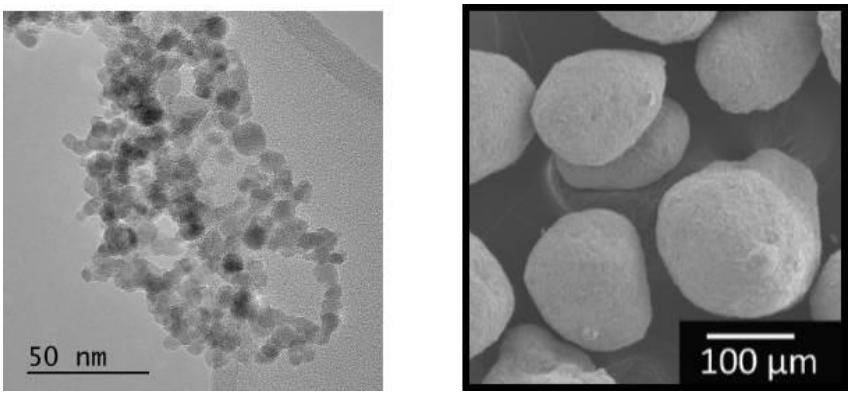

Fig. 1: Manganese oxide micrographs (TEM/SEM) after a) flame spray pyrolysis, and b) after spray granulation.

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