RADICAL UCC AtmoTrace

Symposium

Innovative Measurement Techniques for Trace Gases and Radicals

9-10 January 2025, University College Cork, Ireland

Programme: Day One

Time	Session
11:00-11:15	**Registration** Dora Allman Room, 4th floor, The Hub, UCC
11:15-11:40	**Welcome** Welcome from Sarah Culloty, Head of the College of Science, Engineering and Food Science, University College Cork Introduction to the RADICAL project, Justin Holmes, School of Chemistry Introduction to the AtmoTrace project, Andy Ruth, School of Physics
11:40-13:10	**Session 1:** Spectroscopic techniques for trace gas detection, Chair: Christa Fittschen Markus Sigrist "Photoacoustic trace gas monitoring: a success story" Weidong Chen "Optical monitoring of HO2 radicals using cavity enhanced Faraday rotation approach" Mixtli Campos Pineda "Direct NO3 detection in the Irish Atmospheric Simulation Chamber using Incoherent Broadband Cavity Enhanced Absorption Spectroscopy (IBB-CEAS)" Paul Wills "A new cavity ring-down instrument for airborne monitoring of N2O5, NO3, NO2 and O3 in the upper troposphere lower stratosphere" Eibhlín Halpin "Development of a spectroscopic instrument for measuring real-time nitrogen dioxide concentrations around schools"
13:10-13:20	Group photo in UCC Quad
13:20-14:20	Lunch at UCC Restaurant
14:20-15:40	**Session 2:** Radical atmospheric chemistry with advanced techniques, Chair: John Wenger Christa Fittschen "Atmospheric chemistry studied by Laser Based Techniques"

Brought to you by RADICAL, a Horizon 2020 EIC Pathfinder project developing a low-cost sensor for atmospheric radicals and other gases. RADICAL

In collaboration with AtmoTrace, an SFI Frontiers for the Future Award (Grant Number 21/FFP-A/8973) for the development of ultra-sensitive cavity enhanced trace gas detection techniques. UCC AtmoTrace

The RADICAL project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement number 899282.

Taighde Éireann Research Ireland

	Hendrik Fuchs "Recent advances in instruments for the measurement of hydroxyl radical reactivity" Barbara Nozière "Speciated Detection of Gas-phase Organic Peroxy Radicals and Related Intermediates by Proton Transfer Mass Spectrometry" Neil Donahue "Measuring Peroxy Radicals with a Conversion Inlet and Chemical Ionization Mass Spectrometry"
15:40-16:00	Coffee break
16:00-17:00	**Session 3:** Gas sensors & analytics, Chair: Stig Hellebust Matthew Johnson "Low Cost Sensors for monitoring air pollution in the built environment and pollution control systems" John Saffell "Gas Sensors: Opportunities and Limitations" Donatella Puglisi "Utilization of machine learning in gas sensing for real-world applications"
17:00-17:30	Showcase of UCC's Irish Atmospheric Simulation Chamber Led by John Wenger and Andy Ruth, UCC Kane Building. Optional, limited spaces. Sign up at the registration desk.
19:30	Symposium dinner at Jacob's on the Mall 30 South Mall, Cork. Pre-booked. Check with registration desk for any queries.

Symposium

Innovative Measurement Techniques for Trace Gases and Radicals

9-10 January 2025, University College Cork, Ireland

Programme: Day Two

Time	Session
9:00-9:30	Arrival and coffee Dora Allman Room, 4th floor, The Hub, UCC
9:30-10:45	**Session 4:** Applications of nanomaterials for gas sensing, Chair: Justin Holmes Eduard Llobet Valero "2D materials for gas sensing" Nikol Lambeva "Toward high-sensitivity and low-power consumption gas sensor devices based on 2D transistors" Subhajit Biswas "Silicon and Two-dimensional (2D) flexible devices as next generation gas sensing platform" Vaishali Vardhan "Ambipolar Silicon Nanowire Transistors for Dual-Mode Detection of NO_2 and NH_3 in the Atmosphere"
10:45-11:00	Coffee Break
11:00-12:00	**Session 5:** Chemical interactions and functional materials for gas sensing, Chair: Subhajit Biswas Corrado Di Natale "Porphyrinoids Based Gas Sensors" Victor Chechik "Gas sensing through chemical reactions with organic monolayers" Naeem Iqbal "Ozonolysis of Self-Assembled Alkene Monolayers: A Kinetic and Structural Perspective"

12:00-13:10	**Session 6:** New optical technologies for gas sensing, Chair: Andy Ruth Prince Anandarajah "Gain Switched Optical Frequency Combs for Gas Detection" Jarni Braal "Dual Cavity Dual Comb Interferometry with Incoherent Light" Liam O'Faolain "Micro-Ring Resonator Assisted Photothermal Spectroscopy of Water Vapor" Gabriele Biagi "Investigation of Ammonia Adsorption and Desorption Dynamics in a QEPAS Sensor"
13:10-14:10	Lunch at UCC Restaurant
14:10-15:40	**Round-table discussion on the future of measuring trace gases and radicals** Facilitated by John Wenger and Tamela Maciel, with live drawing from Philip Barrett (Blackshapes)
15:40-15:55	Coffee Break
15:55-16:00	**Event feedback**
16:00-16:30	**Closing remarks**
17:00	Post-event pizza and drinks at Franciscan Well 14A North Mall Cork Optional and at own expense

Book of Abstracts

Session 1: Spectroscopic techniques for trace gas detection, Chair: Christa Fittschen

Markus Sigrist "Photoacoustic trace gas monitoring: a success story"

ETH Zürich, Switzerland

Abstract

During its long history photoacoustic spectroscopy (PAS) has experienced numerous new developments and applications in the field of trace gas monitoring. It has been established as a highly sensitive, robust and easy-to-implement technique. The mid-IR region is preferably used for spectroscopic measurements. Quantum cascade lasers (QCLs), interband cascade lasers (ICLs) and even frequency combs yet also mid-IR LEDs are employed as light sources. PAS gas detection started with conventional – typically acoustically resonant – gas cells of various designs (including multi-pass, Helmholtz, 3D-print, etc.). Later quartz-enhanced PAS (QEPAS) and cantilever-enhanced PAS (CEPAS) schemes were introduced which offer distinguished advantages such as small sampling volumes or higher sensitivity yet also some drawbacks like the high resonance frequency used in QEPAS which requires special attention for gas pressure-dependent measurements and for multi-species detection or gas flow studies in CEPAS applications which may lower the detection sensitivity.

This talk will introduce the basics, instrumentational aspects and novel developments of all these techniques. The performance will be illustrated with several examples. Applications range from well-controlled studies in the lab with sensitivities down to sub-ppt-concentrations to multi-species detection in ambient air either in the field or even from airborne platforms.

Bio

Markus Sigrist is a Professor emeritus at ETH Zürich. His main background is in laser spectroscopic trace gas sensing using techniques like photoacoustics. He authored or co-authored over 200 publications in refereed journals as well as several book chapters and books. He acts as a reviewer for scientific journals and is a member of several societies including Fellow of Optica.

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Taighde Éireann Research Ireland

Weidong Chen "Optical monitoring of HO2 radicals using cavity enhanced Faraday rotation approach"

Université du Littoral Côte d'Opale

Abstract

Radicals play a major role in the atmospheric chemistry, in particular OH and HO2 (hydroxyl and hydroperoxyl radicals) in the daytime: the OH radical is the major oxidant of all trace gases in the atmosphere, and its concentration is closely linked to the HO2 concentration via a rapid recycling of HO2 back into OH through reaction with NO or radical-radical reactions in remote environments. The measurement of their concentration is thus vital to identify a lack in the understanding of gas phase oxidation processes. Current instruments used for the concentration measurements of OH (105–106 molecule/cm3) and HO2 (107–108 molecule/cm3) are mostly very costly, bulky and request calibration and chemical conversion (leading to interferences, in particular for HO2). Many efforts have been made in the last decades to develop optical instruments for direct reliable quantification of both radicals without chemical conversion.

We reported in this talk the development of an instrument based on cavity-enhanced Faraday rotation spectroscopy (CE-FRS) for optical monitoring of HO2 radicals through probing the HO2 lines near 6638.2 cm-1. The experimental detail and preliminary results with a 1σ limit of detection of ~ 7.3×108 molecule.cm-3 for HO2 will be presented and discussed.

Bio

Weidong Chen is full Professor at University of the Littoral Opal Coast (ULCO) in France. His current research interests include: (1) Optical sensing and metrology of trace gases (concentration, isotope ratios, vertical concentration profile) and aerosols (optical properties, mass concentration); (2) Optical parametric laser source generation by frequency conversion.

Mixtli Campos Pineda "Direct NO_3 detection in the Irish Atmospheric Simulation Chamber using Incoherent Broadband Cavity Enhanced Absorption Spectroscopy (IBB-CEAS)"

University College Cork

Abstract
Oxides of nitrogen play key roles in atmospheric chemistry, from the formation of tropospheric ozone to the formation of reactive organic radicals that lead to production of secondary organic aerosol (SOA). The oxidation of volatile organic compounds (VOCs) by the nitrate radical (NO_3) is an important tropospheric process during nighttime that leads to formation of SOA and of alkyl nitrates ($RONO_2$) that can transport NO_2 into less polluted environments. Studying the kinetics of NO_3 is, therefore, important for our understanding of tropospheric chemistry. Direct measurements of NO_3 were performed in the Irish Atmospheric Simulation Chamber (IASC) using IBB-CEAS. The absorption instrument uses an open-path cavity, spanning the full length of the chamber (5 m), in conjunction with a high-power supercontinuum source and a monochromator/CCD assembly. A robust spectral analysis method was developed to retrieve NO_3, NO_2, and H_2O mixing ratios simultaneously form the absorption spectra. The standard deviation of the absorption coefficient for a 10 s integration time was established to be $5x10^{-10}$ cm^{-1}, corresponding to a mixing ratio of ~500 ppqv of NO_3. In this presentation, the detection of NO_3 in different experiments at IASC will be discussed, i.e. from the inorganic NO_y production from NO_2 and ozone, as well as from oxidation of some biogenic VOCs with NO_3 being produced from the thermal decomposition of N_2O_5.

Bio
Mixtli Campos-Pineda is a postdoctoral researcher working in the Irish Atmospheric Simulation Chamber. His focus is the development of spectroscopic techniques for trace gas detection under atmospheric conditions, and the study of oxidation processes of volatile organic compounds.

Paul Wills "A new cavity ring-down instrument for airborne monitoring of N2O5, NO3, NO2 and O3 in the upper troposphere lower stratosphere"

University College Cork

Abstract

A third-generation airfreight container housing 19 different automated instruments from European research partners is being developed currently in order to fly onboard a Lufthansa Airbus 350-900 to monitor ~100 atmospheric trace species in the upper troposphere lower stratosphere (UTLS) – project CARIBIC, www.caribic-atmospheric.com. The first flight is planned for Winter 2025. The air sampled underneath the cargo bay of the aircraft is distributed to all instruments via a dedicated inlet system. All procedures are fully automated and controlled by dedicated electronics and software within the devices. The instrumentation will include a new cavity ring-down (CRD) device from UCC, designed to monitor NO3, N2O5, NO2, and O3. The detection is based on 4 high-finesse optical cavities and 2 diode lasers at 662 and 405 nm for direct absorption detection of NO2 and NO3. O3 and N2O5 are detected on basis of NO titration and thermal decomposition of the sampling gas, respectively.

The chemistry of NO3 and N2O5 is important to the regulation of tropospheric and stratospheric ozone. The in-situ detection of NO3 and N2O5 in the UTLS will help to better understand the nitrogen budget and its influence on ozone transport in this important region of the atmosphere.

In this presentation the measurement principle and technical details of UCC's "CAvity Ring-Down Instrument for Nitrogen Oxide detection" (CARDINO) will be presented along with specifications of this gas sensing device.

Bio

Paul Wills is a PhD student in his second year at University College Cork. He graduated with a BSc in Physics from UCC in 2023. He is a part of the Laser Spectroscopy Group in the School of Physics at UCC.

Eibhlín Halpin "Development of a spectroscopic instrument for measuring real-time nitrogen dioxide concentrations around schools"

Environmental Research Institute, University College Cork

Abstract

Poor air quality can have a serious impact on public health. According to the EPA, air pollution is the cause of over 1,300 premature deaths in Ireland every year. The EPA identified particulate matter (PM) and nitrogen dioxide (NO2) as priority air pollutants for Ireland. This project focuses on NO2, which is a brown gas that is emitted into the atmosphere when fuels are burned, meaning that it is heavily associated with transport emissions. NO2 produces serious health outcomes including an increased risk of cardiovascular mortality, an increased risk of lung cancer, and a 50% increased likelihood of children developing asthma.

NO2 has high spatial and temporal variability, meaning that measuring personal exposure to the pollutant can be challenging. Sensors must be fast, compact, selective and sensitive. Current monitoring systems take a single point measurement, yielding poor spatial resolution, while cheaper, portable sensors do not have sufficient reliability to influence policymakers. This talk will discuss the development of a fast, relatively low-cost NO2 sensor that may also be suitable for public demonstrations. Results showing this spectroscopic technique being tested in the Irish Atmospheric Simulation Chamber (IASC) will be presented. Field measurements of NO2 concentrations near a Cork City primary school will be discussed, identifying peak concentration periods and their causes. Recommendations will be made towards decreasing air pollution around schools.

Bio

Eibhlín Halpin is a PhD researcher at University College Cork (UCC) affiliated with the Environmental Research Institute, specializing in air quality monitoring. Her research primarily focuses on developing cost-effective spectroscopic instruments for detecting nitrogen dioxide in real-time, with the aim to improve pollutant monitoring around schools.

Session 2: Radical atmospheric chemistry with advanced techniques, Chair: John Wenger

Christa Fittschen "Atmospheric chemistry studied by Laser Based Techniques"

CNRS - University Lille

Abstract
Peroxy radicals, RO2, are key species in the atmosphere. They are formed from a reaction of OH radicals with hydrocarbons:
RH + OH + O2 -> RO2 + H2O
In polluted environments, RO2 radicals react predominantly with NO, leading to formation of NO2, and eventually through photolysis of NO2 to formation of O3. At low NOx concentrations such as in the marine boundary layer or the background troposphere, the life-time of RO2 radicals increases and other reaction pathways such as self- and cross reaction with other RO2 or with HO2 radicals become competitive. To study these reactions, UV absorption spectroscopy has been employed in the past: this technique gives good sensitivity for peroxy radicals, but poor selectivity as these radicals all have broad and similar absorption features in the UV.

We have established a technique allowing to follow peroxy radicals with a better selectivity compared to UV, but with still good sensitivity by coupling laser photolysis to cw-Cavity Ring Down Spectroscopy in the near IR. I will present some recent results on measurements of rate constants and branching ratios of the self-reaction of selected peroxy radicals (Assali and Fittschen, 2022a and 2022b, Shamas et al., 2022). Radicals are generated by laser photolysis, and the detection of the peroxy radicals is done be cw-Cavity Ring Down Spectroscopy in the near IR (Zhang et al., 2021), a rather selective method compared to UV absorption spectroscopy.

Bio
Dr. Christa Fittschen is Research Director at CNRS, working at “Physical Chemistry of Combustion and Atmospheric Chemistry Processes” at U of Lille, France. She received PhD in 1989 at University Göttingen under supervision of Prof. Jürgen Troe, did a postdoc from 89-91 at SRI, Menlo Park, CA and is since then in Lille, first 1-year postdoc at Total Oil Company and at CNRS since 1992.

Hendrik Fuchs "Recent advances in instruments for the measurement of hydroxyl radical reactivity"

Forschungszentrum Jülich

Abstract

Hydroxyl radical (OH) reactivity, which is the inverse lifetime of the OH radical, provides information on the burden of air pollutants, since almost all air pollutants react with OH. OH reactivity measurements from field experiments can help to identify gaps in the measurement of individual reactants and serve as a proxy for the potential formation of secondary pollutants, including ozone and particles. In this work, an OH reactivity instrument has been further developed specifically for airborne measurements. The laser system used to detect the OH radicals has been simplified compared to previous setups, thereby significantly reducing the need for user interaction. The high sensitivity of the improved instrument facilitates the data acquisition on board an aircraft as demonstrated by its deployment during the AEROMMA campaign in 2023.

Bio

Since 2022: deputy director of the Institute of Climate and Energy Systems ICE-3: Troposphere, Forschungszentrum Jülich, Germany; since 2021: Professor Physics Department, University of Cologne, Germany; since 2009: Group leader at Forschungszentrum Jülich, Germany; 2007/08: Postdoctoral researcher at NOAA, Boulder, USA; 2006: Ph.D. in physics from Humboldt University Berlin, Germany.

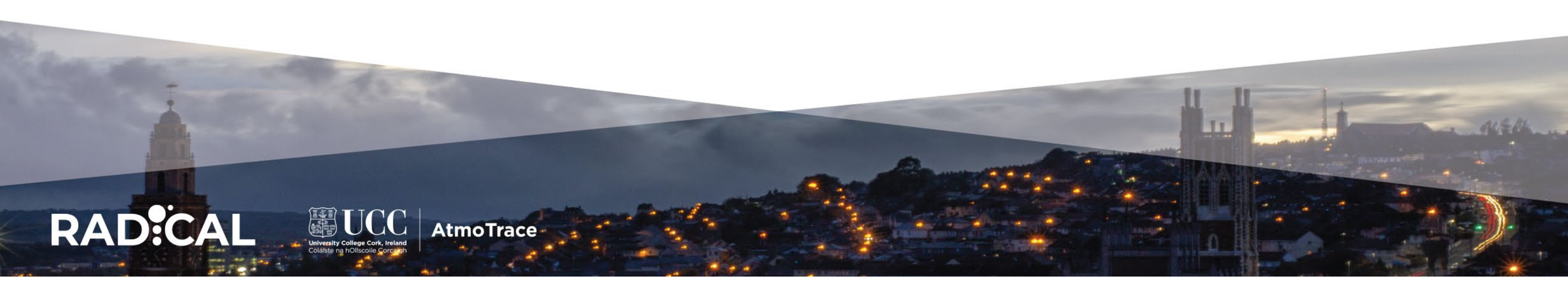
Barbara Nozière "Speciated Detection of Gas-phase Organic Peroxy Radicals and Related Intermediates by Proton Transfer Mass Spectrometry"

KTH Royal Institute of Technology

Abstract
Organic peroxy radicals are important intermediates in nearly all the aerobic chemical systems containing organic compounds, such as living organisms, combustion systems or the atmosphere. In the atmosphere their reactions play important roles in the oxidation cycles and determine whether the oxidation of organic compounds leads to volatile or condensible products. However, few techniques exist to monitor these radicals individually, especially in situ in natural systems.
This presentation will give an overview of a project dedicated to the detection of these radicals using Proton Transfer Mass Spectrometry and aiming at monitoring them in ambient air. Current advances in their detection, the study of their reactions, and the detection of related intermediates will be presented. The main advantages and limits of the technique will be discussed, in particular the specific challenges of determining the absolute concentration of the radicals (calibrations).

Although the technique is still being improved, the results obtained allow already to study new reactions, such as the interactions of the gas-phase radicals with surfaces. They also suggest that this technique could advantageously replace Electron Spin Resonance (ESR) or Electron paramagnetic Resonance (EPR) for some applications in other fields of study than atmospheric chemistry.

Bio
Barbara Nozière is a Professor in physical and atmospheric chemistry at the Royal Institute of Technology (KTH), Sweden. She received her PhD in Physical Chemistry at the University of Bordeaux, France and has been working on the reactivity of organic compounds in the atmosphere since then. One of her interests is the investigation of organic peroxy radicals and their reactions in the atmosphere.



Neil Donahue "Measuring Peroxy Radicals with a Conversion Inlet and Chemical Ionization Mass Spectrometry"

Carnegie Mellon University and University College Cork

Abstract

Peroxy radicals (HO2 and RO2) are central to atmospheric chemistry. The behavior of organoperoxy radicals (RO2) is especially enigmatic and depends strongly on the nature of the R group. During chamber experiments under atmospheric conditions we employ a highly sensitive, medium resolution time of flight mass spectrometer (dTh/Th ~ 10000) to directly measure species with chemical formulas CnHmOy, where m = odd. These are likely RO2. At the same time we employ "HOxROx" chemical conversion in a reactive inlet by adding SO2 and NO. The SO2 converts any OH radicals to H2SO4, and the NO converts HO2 into OH, and indirectly converts (some) RO2 to HO2 and then OH. By simultaneously measuring the CnHmOy species directly and the total RO2 indirectly, and also by observing the CnHmOy behavior with added NO and SO2, we can test how highly substituted RO2 (with high O:C) behave relative to less functionalized RO2 with well known chemistry.

Bio

Neil Donahue is the Thomas Lord University Professor of Chemistry at Carnegie Mellon University. He has a PhD in Meteorology (Atmospheric Chemistry) from MIT and has conducted research into the chemical physics of atmospheric compounds for 40 years.

Session 3: Gas sensors & analytics, Chair: Stig Hellebust

Matthew Johnson "Low Cost Sensors for monitoring air pollution in the built environment and pollution control systems"

Devlabs

Abstract
Low cost sensors are emerging as a powerful new technique for monitoring components of the atmosphere in a variety of environments. New opportunities for monitoring arise due to their low cost, high time resolution and small size, but not without sacrifices in the areas of sensitivity, stability and selectivity [Frederickson, 2019]. I will review our experiences installing networks of low cost sensors for monitoring vertical distribution of roadway pollution [Frederickson, 2024], air pollution in a village [Frederickson, 2022], and, using the world's largest dense network of nodes, monitoring air pollution for two years at 225 locations in the Borough of Camden in London at 3 min intervals [Bogaert, 2024]. In addition we have worked with personal exposure monitoring for professional drivers [Frederickson, 2020], users of the Copenhagen Metro [Kappelt, 2023], and pedestrians in Copenhagen [Frederickson, 2023]. Finally we have used the sensors to monitor the impact of alternative green processes at a building site in Aarhus Denmark, to reduce noise, particulate and NO2 pollution. In addition we use low cost sensors as part of innovative new pollution control systems. The system being deployed by Luper Tech in the Netherlands uses the hydroxyl radical to remove odor from wastewater treatment systems [Johnson, 2014], and the system being tested by Ambient Carbon uses chlorine atoms to destroy methane from low concentration sources like dairy barns [Krogsbøll, 2023].

Bio
Matthew Johnson is Professor of Chemistry at Uni Copenhagen with BA from Macalester College and PhD from Caltech. Research on kinetics, spectroscopy, atmospheric chemistry and innovation. He is coauthor of 151 publications, 12 patents and two books. He has a role as founder, CSO, CEO in startup companies including Infuser, Airlabs, Airscape, Rensair, Devlabs, Luper Tech and Ambient Carbon.

John Saffell "Gas Sensors: Opportunities and Limitations"

NosmoTech Ltd.

Abstract

Low cost gas sensors rely mainly on three technologies: amperometric electrochemical cells, chemiresistive metal oxides and non-dispersive infrared (NDIR) absorption, each with their advantages and limitations.

Advances in catalysts and electrolytes, driven by the move to EV transport, control of material morphologies at the nano scale and high volume laser diodes with polymer optics have opened opportunities to improve sensitivity, stability and selectivity for all three technologies.

Electrochemical gas sensors dominate the industrial safety market and have now entered the air quality industry, with sensitivity around 5-10 ppb. Improved filters, alternative electrolytes, 4-electrode configurations and novel catalysts are being developed, targeting better long term stability and useful VOC selectivity.
Metal oxides, known for low cost and durability are trying to improve sensitivity, selectivity and baseline stability. Integrating both n-type and p-type sensing layers onto microhotplate arrays is beginning to produce lower power, more stable sensor arrays. Edge computing using ML and AI will hopefully improve selectivity, and heterogenous nano-controlled sensing layers should rid us of humidity dependence and baseline drift.

NDIR cells have profited from the new NIR and mid-IR LEDs with power now regularly below 2mW (rms). Extending into the mid-IR and even looking at NDUV are showing promise for specific VOCs such as formaldehyde.
The future looks bright, if we are smart.

Bio

John Saffell has a BSc in Chemistry and a PhD in Materials Science. He founded Solomat Ltd, in 1979, developing air and water quality instrumentation. In 1997 he co-founded and was Technical Director of Alphasense until 2021, developing low cost gas and particle sensors. He is Chairman of CoGDEM and a Director of NosmoTech Ltd, consulting in air quality and developing IAQ sensor networks.

Donatella Puglisi "Utilization of machine learning in gas sensing for real-world applications"

Linköping University

Abstract
Today’s challenges and demands for smart, portable, and price-competitive gas sensor systems require the development of novel solutions capable of achieving not simply incremental improvements, but a true paradigm shift of the current state-of-the-art in gas sensing technologies and applications. Despite several decades of research and development of novel sensing materials and intelligent operating modes, chemical gas sensors still suffer from poor selectivity, signal drift, influence of humidity, temperature, and other environmental parameters, among other problems, resulting in lack of accuracy and reliability of measurement readings. Here, we show that chemical gas sensors combined with machine learning are finally mature enough to accelerate innovation and application in a variety of new real-world scenarios. The Nobel Prize in Physics 2024 is clear evidence of the crucial role of machine learning for unprecedented advancements in science and technology as well as for our daily lives. To support our arguments and facilitate understanding, we provide practical examples and case studies in air quality and environmental monitoring, meat inspection, forensic sciences, and cancer diagnostics.

Bio
Donatella Puglisi, Associate Professor of Applied Physics at Linköping University, Sweden, specializes in gas sensing devices and digital technologies for a variety of applications focused on volatile organic compounds. She is also a qualified educator and course designer. Her contributions to technology transfer, networking, and community engagement underscore her commitment to societal impact.

Leonidas Tsetseris "Computational studies on the detection of atmospheric radicals and gases"

National Technical University of Athens
Unable to present due to travel disruption

Abstract
So-called ab initio calculations within the Density Functional Theory (DFT) approach has long been an indispensable tool in materials modelling. By providing accurate solutions to the quantum mechanical equations that govern the dynamics of electrons, DFT calculations are recognized as the most efficient and reliable method to elucidate key properties of materials which are used in a wide range of state-of-the-art or emerging technologies. This talk will present results and findings of extensive DFT studies on the detection of atmospheric hydroxyl and nitrate radicals, as well as of other important molecular species, such as ozone, nitrogen dioxide and ammonia. In close collaborations with experimental partners within the RADICAL project, the computational studies have probed key issues related to gas sensing, such as the nature of adsorption (physisorption or chemisorption) on suitable substrates (e.g. on silica-covered Si-based nanowires, or on two-dimensional materials), the energetics and kinetics of radical-induced reactions, and the formation of charge carrier traps which can alter the characteristics of pertinent electronic devices (enabling thus the sensing of radicals and molecules).

This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement number 899282 — RADICAL — H2020-FETOPEN-2018-2020 / H2020-FETOPEN-2018-2019-2020-01.

Bio
Leonidas Tsetseris is a Professor of Physics at the School of Applied Mathematical and Physical Sciences of the National Technical University of Athens (Greece). His research focuses on the computational modelling of materials which are suitable for a wide range of technologies, such as photovoltaics, electronics, laser-induced printing and sensors.

Session 4: Applications of nanomaterials for gas sensing, Chair: Justin Holmes

Eduard Llobet Valero "2D materials for gas sensing"

Universitat Rovira i Virgili

Abstract
Having affordable, power-lean, highly sensitive and selective gas sensors is essential to enable the widespread and continuous monitoring of air pollutant and toxic gases. In the last years the research community has identified two-dimensional nanomaterials as having high potential for developing a new generation of room-temperature operated devices for detecting gases and vapours at trace levels in the ambient. My talk reviews some recent developments, identifies current shortcomings where breakthroughs are most needed, and discusses aspects where research efforts should be put to overcome the main difficulties experienced. These efforts range from gaining more insight in the gas sensing mechanisms to ameliorating the synthesis and processing of 2D nanomaterials for better controlling surface, interface and edge chemistry and defects.

Bio
ICREA Academia Professor at the University of Tarragona (Catalonia, Spain). President of the Spanish Research Network on Microsystems and Nanotechnology. Founder of two spin-off companies. With research interests in the growth of nanomaterials for gas sensing, photocatalysis and energy and the study of their working principles.

Nikol Lambeva "Toward high-sensitivity and low-power consumption gas sensor devices based on 2D transistors"

Helmholtz-Zentrum Dresden-Rossendorf

Abstract
In recent years, two-dimensional (2D) materials have shown significant advancements in fundamental properties, making them valuable for energy harvesting, storage, and optoelectronics applications. Notably, 2D materials have emerged as promising candidates for gas sensing technology due to their high surface-to-volume ratios and active surface sites, which enhance gas molecule absorption and sensitivity. This improved sensitivity could overcome the limitations of conventional sensors in detecting low gas concentrations and reducing power consumption. Furthermore, the small size, flexibility, and low power requirements of 2D-based gas sensors make them ideal for portable devices and Internet of Things (IoT) applications where energy efficiency is essential.

Among 2D materials, black phosphorus (BP) has gained significant attention for gas sensing thanks to its layered structure and strong chemical reactivity. In this presentation, we will review advanced gas-sensing devices based on 2D materials, focusing on their main operational principles. We will also highlight recent developments in our group, particularly the fabrication of field-effect transistors (FETs) as gas sensors. Specifically, we will discuss using BP-FET sensor devices for detecting CO2 and other gases.

Bio
Nikol Lambeva is a researcher in the Department of Nanoelectronics at Helmholtz-Zentrum Dresden-Rossendorf. She earned her PhD from the University of Oxford, focusing on conjugated organic polymers for LED applications. Her current research explores structure-property relationships in advanced materials for next-generation devices, focusing on 2D material systems for sensing applications.

Subhajit Biswas "Silicon and Two-dimensional (2D) flexible devices as next generation gas sensing platform"

University College Cork

Abstract
This talk will explore three distinct sensing platforms developed within the "RADICAL" project. To begin, we'll showcase 2D Molybdenum sulphide (MoS_2) sensors created through electrochemical exfoliation, ink production, and printing techniques for detecting NO_2 at parts-per-billion levels. These sensors demonstrated reliable detection across a broad spectrum of NO_2 concentrations, spanning from 100 ppb to 50 ppm, underscoring the significant potential of room-temperature MoS_2-based NO_2 sensors. Density functional theory (DFT) calculations reveal that these electrochemically exfoliated MoS_2 sensors surpass their mechanically exfoliated counterparts due to their abundant surface defects and vacancies. Next, we'll discuss our development of highly efficient ambipolar silicon junction-less nanowire transistors (JNTs) featuring a unique dual reaction for identifying both oxidative NO_2 and reductive NH_3 pollutants. Various Si-JNT characteristics exhibited dynamic shifts on both p- and n-sides of the ambipolar transistor devices when exposed to NO_2 across a wide concentration range (250 ppb-50 ppm), resulting in a dual response. Lastly, we'll present our recently developed sensor platform utilizing molecular modified Schottky junctions with organic monolayer for instantaneous detection of gaseous ozone and hydroxyl radicals at ambient temperature. This innovative platform enables accurate identification of ozone and hydroxyl radicals within a concentration range of 1 ppb to 1 ppm.

Bio
Dr. Subhajit Biswas is a Senior Researcher in the School of Chemistry at University College Cork. His research expertise includes semiconductor nanomaterials and devices, bottom-up fabrication, gas sensing, and materials for energy storage and harvesting. Dr. Biswas has published his research on these topics in prestigious journals such as Nature Physics, Nature Communications, Nano Letters etc.

Vaishali Vardhan "Ambipolar Silicon Nanowire Transistors for Dual-Mode Detection of NO_2 and NH_3 in the Atmosphere"

University College Cork

Abstract
Our work presents a study on ambipolar silicon junction-less nanowire transistors (Si-JNTs) demonstrating significant sensitivity to oxidative pollutants, specifically nitrogen dioxide (NO_2) and ammonia (NH_3). The ambipolar Si-JNTs display distinct dual responses, altering key electrical characteristics, including on-current (I_{on}), threshold voltage (V_{th}), and mobility (μ), in response to varying concentrations of NO_2 and NH_3 across a wide range (250 ppb to 50 ppm). These Si-JNT devices leverage their high surface-to-volume ratio, chemical interaction capability, and room temperature operation to achieve enhanced sensing performance. By acting as pseudo dopants, NO_2 and NH_3 influence the ambipolar properties of the devices, modifying the behaviour on both p-type and n-type sides. This dual-response mechanism enables selective and versatile sensing of gases, highlighting the potential of Si-JNTs as a single-device solution for effective, highly sensitive, and selective gas detection.

Bio
Vaishali Vardhan is a PhD student at the School of Chemistry, University College Cork.

Session 5: Chemical interactions and functional materials for gas sensing, Chair: Subhajit Biswas

Corrado Di Natale "Porphyrinoids Based Gas Sensors"

University of Rome Tor Vergata, Department of Electronic Engineering

Abstract

The properties demonstrated by porphyrins in natural systems have inspired the use of these molecules for chemical sensors. The interaction of porphyrinoids with gas molecules involve several mechanisms including hydrogen bond, Van der Waals forces, and coordination. Coordinating molecules have a preferential absorption, however the response to other molecules is not negligible, thus porphyrin sensors are seldom selective. The pattern of sensitivity strongly depends on changes in the molecular structure. This facilitates the design of sensor arrays implementing the combinatorial selectivity of olfaction. The low conductivity of porphyrins prompted their use with mass sensors such as quartz microbalances. These sensors were used to prepare electronic noses for various applications, not least medical diagnosis from the analysis of volatile metabolites. Despite their positive features, quartz microbalances are bulky and costly devices not suitable for miniaturization. Thus, the challenge is the development of impedance-based sensors that can preserve the results obtained with mass sensors. To this regard, we have been interested to study the combination of porphyrnoids with inorganic, and organic semiconductors. Interesting results are obtained with ZnO nanostructures and with porphyrinoids polymers. The sensitivity of these devices approach that of quartz microbalance sensors paving the way for a large-scale deployment of porphyrinoids based artificial olfaction systems.

Bio

Corrado Di Natale is full professor of Electronics at the University of Rome Tor Vergata and director of the Interdepartmental Centre for Volatilomics “A.D’Amico”. His research interests span from the development of chemical sensors and biosensors to integrated artificial sensorial systems (olfaction and taste) and their use in environmental, medical and food applications.

Victor Chechik "Gas sensing through chemical reactions with organic monolayers"

University of York

Abstract
Gas sensing is usually based on reversible interactions between the analyte molecules and the sensor surface. However some molecules (e.g., OH radical) are highly reactive and will react irreversibly with almost any organic material. Chemical detection of such species can be done through reactions with an organic coating on the sensor surface. Although this method has significant disadvantages (e.g., following a complete reaction of the surface functional groups the sensor needs to be replaced), it enables chemical detection of otherwise elusive species.

Developing such a reaction-based sensor requires good understanding of the mechanistic features of reactions at the gas-solid interface. For instance, the reactivity of molecules in a monolayer can be different from the bulk phase, and can depend on the degree of packing, and the accessibility of functional groups potentially buried within the monolayer. The reaction pathways could be affected by the high concentration of the sensing molecules in the monolayer and limited mobility of surface-attached functionalities.

We used an alkene ozonolysis reaction as a model system to probe such mechanistic features of surface chemistry. The results suggest that the monolayer reactivity parallels that in the bulk phase, but the product distribution is different from the reactions in the homogeneous phase (e.g., gas phase).

Bio
Victor Chechik is a mechanistic organic chemist with particular interests in free radical chemistry and reactivity in supramolecular systems (including organic monolayers). After completing his PhD in St Petersburg and postdoctoral research in Sheffield (UK) and Texas A&M University (US), he joined University of York in 2000 and has been there since.

Naeem Iqbal "Ozonolysis of Self-Assembled Alkene Monolayers: A Kinetic and Structural Perspective"

University of York

Abstract

Interfacial reactions play an important role in material science particularly due to their applications in electronics and sensing. Understanding the underlying mechanism of surface reactions provides crucial information for fundamental studies in sensor development. The interfacial reaction between ozone and alkenes has been studied extensively due to its importance in atmospheric chemistry, sensing, and coatings however, the structure-activity relationship for such surface reactions has been less explored. This study investigated the ozonolysis of a series of self-assembled alkene monolayers on solid supports with different chain lengths, regiochemistry, and mixed monolayers. Glass slides and non-porous silica nanoparticles were used as model surface supports. The organic surfaces were characterized using different spectroscopic techniques (NMR, IR) and contact angle measurements. A decrease in the contact angle of the surfaces was observed and the formation of secondary ozonide was confirmed with the help of solid state ^{13}C NMR after the ozonolysis reaction. The kinetics of ozonolysis was studied by monitoring the change in contact angle over time. Kinetic data suggested that the rate of ozonolysis is almost independent of the chain length although the alkene with the shortest 4-carbon chain reacted slightly faster. The internal 8-carbon alkene reacted at a faster rate than the terminal alkene in agreement with the bulk reactivity trends.

Bio

Naeem Iqbal is an organic chemist specializing in methodology development and the synthesis of target molecules. His current research focuses on surface functionalization and interfacial reactions, including ozonolysis. With extensive expertise in characterizing organic molecules, he leverages advanced techniques to monitor and understand complex interfacial processes for scientific and practical applications.

Session 6: New optical technologies for gas sensing, Chair: Andy Ruth

Prince Anandarajah "Gain Switched Optical Frequency Combs for Gas Detection"

Dublin City University (DCU)

Abstract

Optical frequency combs (OFCs) and their implementation were well documented by early reports in the 60's and 70's including the Nobel lecture by Hansch and Hall. Of recent, there has been an enormous amount of research activity focusing on OFC generation, characterisation and their wide range of applications including molecular spectroscopy, astronomy, RF photonics, optical clocks, arbitrary waveform generation, and optical communications. An OFC can be defined, as a series of equally spaced discrete spectral lines. There are various parameters that could be used to characterise an OFC, and the choice of optimum ones depend on the nature of the application. The talk will look at the pros and cons of the many different techniques available to generate an OFC and focus on gain switching of commercially available semiconductor lasers due to its simplicity and flexibility. Shortcomings associated with gain switching and methods to overcome them, particularly using external optical injection locking (OIL) will be assessed.

Finally, the talk will address how gain switched dual comb spectroscopy (DCS) can be used to overcome many of the constraints of conventional Fourier transform infra-red spectroscopy through the simplification of the receiver, offering high precision, short acquisition times and potentially low bandwidth detectors. Exemplar experiments on the detection of gases such as H2S and NH3 will be discussed.

Bio

Dr Prince Anandarajah is currently an associate professor in the School of Electronic Engineering at DCU. His main research interests include high speed optical communications and photonic sensing. He has published over 240 articles and 7 international patents. He is also a founder and a director of Pilot Photonics (a spin-off company). He is a senior member of the IEEE.

Jarni Braal "Dual Cavity Dual Comb Interferometry with Incoherent Light"

University College Cork & Environmental Research Institute

Abstract

In recent years, applications using two phase coherent frequency combs have attracted great interest in the field of molecular spectroscopy and trace gas sensing. In Dual Comb Spectroscopy (DCS) two frequency combs produce a time dependent interferogram on a detector after passing through a gas sample. This interferogram can be Fourier transformed to extract high resolution optical spectra using a single photodetector.

Using DCS in conjunction with optical cavities for enhanced absorption sensitivity, however, has proven challenging due to the difficulties in matching frequency combs to the mode structure of high finesse cavities, which requires stable active electronic locking schemes. In contrast Dual Cavity Dual Comb Interferometry (DC-COIN) is a novel method using a high intensity broadband incoherent light source to generate interferograms analogous to DCS by combining the light transmitted by two optical cavities with slightly different free spectral ranges. It allows a spectrum to be obtained with a single detector, with high resolution and high sensitivity.

In this presentation we show that using incoherent NIR light (1540-1560 nm) from a spectrally filtered and amplified superluminescent light emitting diode enables the detection of CO_2, C_2H_2, and H_2O with a resolution of ~306 MHz with DC-COIN. Proof-of-principle measurements will be presented and pros and cons of the DC-COIN approach for next generation gas sensing will be discussed.

Bio

Jarni Braal is a 4th year PhD student at University College Cork (UCC). During a joint Industrial Physics BSc at UCC and Munster Technological University he worked on Z-Stacking and deconvolution algorithms at the Centre for Advanced Photonics & Process Analysis. After graduation Jarni joined the laser spectroscopy group in UCC to develop new and innovative methods for trace gas sensing.

Liam O’Faolain "Micro-Ring Resonator Assisted Photothermal Spectroscopy of Water Vapor"

Munster Technological University

Abstract
We will present the development of micro-ring resonator (MRR) assisted photothermal spectroscopy (PTS) for gas phase samples, focusing on water vapor detection. Micro-ring resonators, particularly silicon nitride-based ones, offer high finesse and potential for miniaturization in silicon photonics, enabling mass production and compact design. The study demonstrates the use of a telecommunications wavelength probe laser and a 1395 nm diode laser to excite and measure the photothermal effect in water vapor, which is relevant to various fields such as industrial process monitoring, medical gas quality control, and environmental research.

Traditional moisture sensors, such as capacitive and resistive sensors, face limitations of cross-sensitivity to other substances and limited dynamic range. While diode laser absorption spectrometers offer high selectivity, their size restricts their use in inline sensing applications. We show that integrated PTS-based gas sensors could address these challenges by offering high selectivity with a small footprint, making them suitable for various applications. This research marks the first step towards developing such advanced sensor technology.

Bio
Liam O’Faolain leads the Nanophotonics Group at MTU’s Centre for Advanced Photonics and Process Analysis. His research focuses on power-efficient lasers and innovative sensors using integrated photonics and Nanophotonics. He has authored over 120 papers and coordinates several major projects, including EVOQUE, METASPECS, PROTEMIC, and PASSEPARTOUT. His h-index is 50.

Gabriele Biagi "Investigation of Ammonia Adsorption and Desorption Dynamics in a QEPAS Sensor"

Munster Technological University

Abstract
Ammonia monitoring is critical for various agricultural, industrial, and environmental applications due to its significant role in fertilizers and potential environmental and health impacts. In recent years, quartz-enhanced photoacoustic spectroscopy (QEPAS) sensors have been widely utilised for the development of ammonia trace sensors. However accurate monitoring systems face challenges due to ammonia's strong tendency to interact with the surfaces. This study aims to characterize the adsorption and desorption dynamics of ammonia in a QEPAS sensor employing a thermoplastic polyurethane (TPU) tube system and a laser diode targeting the NH_3 adsorption line at 1531.65nm (6528.90 cm^{-1}) with an optical power of 35.2 mW. The internal wall surface of a sensor and tubes can be considered as a place with free binding sites for NH_3 molecules thereby constituting a reservoir of molecules. In this experiment, ammonia mixtures of varying concentrations were flushed through the QEPAS sensor to determine the gas-exchange time constant, as well as the adsorption and desorption time constants. Furthermore, under non-dry gas conditions, the presence of water vapour affects the processes. To ensure the accuracy of the results, a capacitive humidity and temperature sensor is integrated into the gas line, enabling the real-time monitoring of both the water vapour concentration and the gas temperature.

Bio
Gabriele is completing his PhD project focused on the development of compact sensors to detect NH_3, CH_4, and CO_2. This Marie-Curie project is part of a collaboration between the MTU and the PolySenSe lab at UNIBA. Additionally, he is involved in the European Project APP4FARM which aims to understand the complex dynamics of soil ecosystems using a novel optical gas monitoring system.