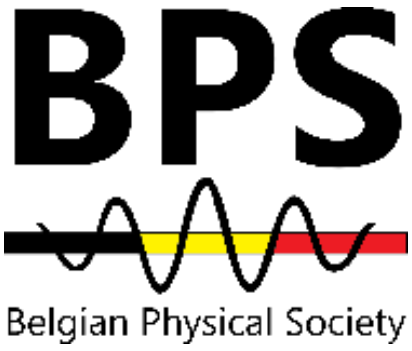
Belgian Physical Society

Belgische Natuurkundige Vereniging

Société Belge de Physique

General Scientific Meeting 2022

Book of abstracts



Tabloo, Gravenstraat 3, 2480 Dessel – May 18, 2022

https://www.belgianphysicalsociety.be/

Organizing Committee

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BPS General Scientific Meeting

May 18, 2022 – Tabloo, Gravenstraat 3, 2480 Dessel

	Tabloo central court and exhibition				
09:30 h	Welcome coffee and registration				
09:30 h	Poster session and possibility to visit Tabloo Expoo (group 1)				
	Room Neutron	**Room Alfa and Beta**		**Room Laboo**	**Room Proton**
	Plenary session – Chair: Jef Ongena (BPS, ERM-KMS)				Posters
10:45 h	Welcome – Jef Ongena / Michèle Coeck				
11:00 h	Nuclear fission – un unexpected charm, an inexhaustible wealth Eric van Walle (SCK CEN)				
11:40 h	Nuclear fusion research in Belgium and Europe: status and latest results Yevgen Kazakov (ERM-KMS)				
12:20 h	Exoplanets or the quest for other worlds Michaël Gillon (University of Liège)				
13:00 h	Walking lunch and poster session				
13:30 h				**Tabloo for teachers**	Posters
14:00 h	**Young Speakers Contest – Chair: Fabrice Louche (ERM-KMS)** • Marine De Clerck (VUB) • Matthew Houtput (UAntwerp) • Orazio Zapparata (ULB)			13:30 h Introduction to Tabloo and practical information for school visits 14:00 h Visit Tabloo Expoo or join the BPS programme: YSC and Education session	
	Physics session – Chair: Michaël Lobet (UNamur)	**Education session – Chair: Michèle Coeck (SCK CEN)**			
15:15 h	Materials design through ensemble learning: when the average model knows best – Danny E.P. Vanpoucke (UHasselt)	15:15 h	SCK CEN Academy's STEM initiatives and perception study on nuclear science and technology – Lisanne Van Puyvelde (SCK CEN)		
15:35 h	Inverse atmospheric transport modelling for identifying Nuclear-Test-Ban Treaty violations – Pieter De Meutter (SCK CEN)	15:30 h	Artificial intelligence for materials industry: an open online course – Michaël Sluydts (UGent)		
15:55 h	Transparent for humans, visible for birds: UV-reflecting coating for bird-safe window – Sébastien R. Mouchet (UNamur, University of Exeter)	15:45 h	Online learning that is worth it in a post-pandemic world - Stefaan Cottenier (UGent)		
16:15 h	Break	16:00 h	Workshop on Problem Based Learning Katleen Denolf (UHasselt)		
16:45 h	Planetary states of the Sr atom – Matthieu Génévriez (UCLouvain)				
17:05 h	Growth mechanisms of CVD Diamond – Emerick Guillaume (UHasselt, IMOMEC)				
17:30 h	Reception and poster session Possibility to visit Tabloo Expoo until 20:00 h (group 2)				
20:00 h	Closure				

Sponsored by:

Oral presentations

Nuclear fission – un unexpected charm, an inexhaustible wealth

Eric van Walle
Belgian Nuclear Research Centre (SCK CEN), Mol

eric.van.walle@sckcen.be

Abstract

Nuclear fission was a very unexpected discovery that lies at the basis of neutron physics and applications. Neutron driven nuclear reactors were soon available and were source to electricity production that changed the life of many citizen especially in the western hemisphere. Due to several nuclear accidents and the downside of creating nuclear waste, the further development of nuclear power plants based on fission was delayed, but today we see an upcoming trend that moves in the direction of fast reactors and small modular reactors with the geographical center of development being displaced.
This presentation will give a broad overview of fission related applications and will demonstrate that the game ain't over yet!

Nuclear fusion research in Belgium and Europe: status and latest results

Yevgen Kazakov
Laboratory for Plasma Physics, LPP-ERM-KMS, Brussels

kazakov@chalmers.se

Abstract

The urgent need for environmentally friendly energy sources becomes increasingly more important. Among several options, nuclear fusion holds the promise as a safe, clean and almost inexhaustible energy source to fulfill our long-term energy needs [1]. In this talk, we review the fundamental concepts of nuclear fusion and focus on the two lines of magnetic confinement fusion devices pursued in Europe: tokamaks and stellarators. Encouraging results will be given that highlight the recent significant advances in fusion science and technology. In particular, we will present the latest findings obtained at the world-largest tokamak JET (Culham, UK) [2], including the identification of novel heating scenarios and their applications [3, 4], and key results of the recent D-T campaign in the second half of 2021. We will also discuss main findings from the world-largest stellarator Wendelstein 7-X (Greifswald, Germany) such as the experimental demonstration of the optimization of its magnetic geometry for minimizing neoclassical heat losses [5]. This is followed by a discussion of the status of the next-step international ITER project in France and plans for the demonstration fusion power plant DEMO. The talk will also highlight recent achievements and key contributions of the Belgian Fusion Association to international fusion research.

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Exoplanets or the quest for other worlds

Michaël Gillon
University of Liège

michael.gillon@uliege.be

Abstract

Initiated in the XVIth century, the Copernican revolution toppled our Earth from its theological pedestal, progressively revealing it not to be the center of everything but a planet among several others in orbit around one of the zillions of stars of our Universe. Already proposed by some philosophers at the dawn of this major paradigm shift, the existence of exoplanets, i.e. planets in orbit around other stars than our Sun, remained suspected but unconfirmed for centuries. It is only in the last decade of the XXth century that the first of these extrasolar worlds were found. Their seminal discoveries initiated the development of more and more ambitious projects that led eventually to the detection of thousands of exoplanets, including a few dozen potentially habitable ones, i.e. Earth-like exoplanets that could harbor large amounts of liquid water -and maybe life- on their surfaces. Our most powerful telescopes will soon be able to probe the atmospheric compositions of some of these extrasolar worlds, performing maybe in the process the historical detection of chemical signs of life light-years away. Such a discovery would change our view of the Cosmos forever.

Complexity in integrable and chaotic quantum systems

Marine De Clerck
Vrije Universiteit Brussel, Brussels

Marine.Alexandra.De.Clerck@vub.be

Abstract

The complexity of a computational process is a central notion in information theory. In fact, one can regard any physical process as a computation with an associated complexity, and it is an interesting perspective to characterize motion through the complexity of its dynamics. In particular, the structure present in integrable models generally suggests them to be fundamentally 'simpler' than chaotic motion, and this is expected to be reflected in the complexity of the associated dynamics.
In quantum information theory, complexity is defined in terms of the minimal number of simple operations ('quantum gates') one can apply to approximate a given unitary operator. However, computing the complexity of continuously evolving physical systems requires a generalization of this notion. One such generalization was provided by Nielsen, who proposed to define the complexity of a unitary operator by the length of the shortest path connecting this unitary to the identity operator on the manifold of unitary operators. This notion of complexity requires a set of choices to define the metric on the manifold of unitaries and it is instructive to ask whether Nielsen's complexity distinguishes between integrable and chaotic dynamics irrespective of these choices.
In recent work, we addressed the difference between integrable and chaotic motion in quantum theory as manifested by Nielsen's complexity of the corresponding evolution oper- ators. Complexity is understood here as the shortest geodesic distance between the time- dependent evolution operator and the origin within the group of unitaries. An appropriate 'complexity metric' must be used that takes into account the relative difficulty of performing 'nonlocal' operations that act on many degrees of freedom at once. While simply formulated and geometrically attractive, this notion of complexity is numerically intractable save for toy models with Hilbert spaces of very low dimensions. To bypass this difficulty, we trade the exact definition in terms of geodesics for an upper bound on complexity, obtained by minimizing the distance over an explicitly prescribed infinite set of curves, rather than over all possible curves. Identifying this upper bound turns out equivalent to the closest vector problem (CVP) previously studied in integer optimization theory, in particular, in relation to lattice-based cryptography.
We estimate the solution to the CVP by utilizing approximate algorithms provided by the existing mathematical considerations, resulting in a tightening of the upper bound on quantum evolution complexity. We find that our complexity bound systematically assigns lower values to integrable than to chaotic systems, as we demonstrate by explicit numerical work for Hilbert spaces of dimensions up to ~ 104.

Beyond the Fröhich Hamiltonian: Large polarons in anharmonic solids

M. Houtput and J.Tempere
University of Antwerp, Antwerp

Matthew.Houtput@uantwerpen.be

Abstract

A conduction electron moving in a polar crystal can interact with the lattice vibrations, an effect known as electron-phonon coupling. Usually, the electron and phonon cloud are combined into a new quasiparticle, called the polaron. Electron-phonon coupling is often described using the Fro¨hlich Hamiltonian [1] because of its relative simplicity. This Hamiltonian assumes a linear electron-phonon interaction, but in recent years significant interest has been raised in additional interaction terms. In particular, phonon-phonon in- teractions are important in strongly anharmonic materials such as hydrides under extreme pressures [2], and 1-electron-2-phonon interaction has been proposed to understand sev- eral key properties of strontium titanate [3]. In our work, we extend Fro¨hlich theory to include both of these interactions and investigate the properties of the resulting polaron. Our key result is an analytical expression for the interaction strength of an electron cou- pling to 2 LO phonons in the continuum approximation. For cubic materials, the in- teraction strength only depends on a single scalar parameter, making it well-suited for analytical calculations [4].
Using the resulting Hamiltonian, we calculate the binding energy and effective mass of the new polaron. Since the resulting Hamiltonian is quadratic, the path integral formalism can be used to obtain a variational upper bound valid at all coupling strengths. It is shown that the additional term may significantly lower the polaron's ground state energy and significantly increase its effective mass. It is also shown that the optical absorption spectrum of the polaron shows a characteristic second peak when 1-electron-2-phonon interaction is present, which can be used as an experimental fingerprint to determine how strong this interaction is. Finally, the possibility of bipolaron formation in this extended model is investigated, and it is shown that the beyond-Fro¨hlich interaction significantly broadens the bipolaron stability regime.

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Time dependent detector simulations for deep learning algorithms applied in the study of the origin of ultra high energy cosmic rays

Orazio Zapparrata (for the Pierre Auger collaboration)
Université Libre de Bruxelles, Brussels

Orazio.Zapparrata@ulb.be

Abstract

Ultra high energy cosmic rays are particles with energies that can exceed 1020 eV and are messengers of the most violent phenomena in the Universe. As one of the tools of the emerging Multi-messenger Astronomy, cosmic rays can reveal information about extra-galactic sources and the processes that are taking place in those extreme environments.
The Pierre Auger Observatory is the largest experiment ever built capable of detecting these air-showers and to infer properties of primary cosmic-rays with energies above 1017 eV. The Observatory combines different detectors: fluorescence detectors, a surface array composed of 1660 water-Cherenkov detectors, radio antennas, buried muon detectors and most recently scintillators.
One of the main goals is to establish the composition of these energetic particles to unveil their origin by identifying a sub-sample of cosmic rays that contains a large fraction of a light component (low charge) that is less deflected by galactic and extra-galactic magnetic fields. The nuclear mass composition of these particles is currently obtained using fluorescence detectors that are limited to dark and moonless nights, reducing statistics. The Surface Detector (SD), however, has an almost 100% duty cycle but is not able to directly measure the mass composition. Deep learning methods can allow the determination the mass composition from the SD data with good accuracy, increasing the statistics and the energy range.
The Observatory started the data taking in 2004 and has operated for more than 20 years. Therefore aging effects of the water Cherenkov detectors (WCD) started to appear in the acquired data. However no time dependent detector simulations have been ever produced. We started to address this problem by studying the dependency of the detector response using Geant4 simulations that take into account possible deteriorations of intrinsic characteristics of the water-Cherenkov tanks, such as the water quality and/or their internal optical properties (reflectivity).
The time decay constant of calibration signals was used to compare data and simulations over time and model the aging and the loss of signals.
Our model is able to describe the evolution over time of the recorded signals for all the 1660 stations by decreasing the internal reflectivity of the tanks by 1.7% over 15 years of operations. This provides us with a robust tool to address this evolution over time,fine-tune high-level analysis and it represents a first step towards enabling the production of more reliable time-dependent simulations which will also improve the current and future systematic uncertainties in the data analysis.
A better description of the surface detector will allow us to improve the potential of deep learning algorithms, that require a very good matching between data and the simulations used for the training.

Materials design through ensemble learning: when the average model know best

D. E. P. Vanpoucke[1], O. S. J. Van Knippenberg[2], K. Hermans[2], S. Mehrkanoon[3], and K. V. Bernaerts[4]
[1] Hasselt University, Diepenbeek
[2] CCL Olympic B.V., Venray, The Netherlands
[3] Maastricht University, Maastricht The Netherlands
[4] Maastricht University, Geleen, The Netherlands

Danny.Vanpoucke@UHasselt.be

Abstract

Machine Learning plays an ever more important role in modern materials-design and- discovery presenting a steady flow of new discoveries. Unfortunately, these achievements are generally rooted in large data sets. Although such big data sets are becoming more common place, they are generally not representative for the day-to-day work performed by materials researchers, where large numbers of samples are often unfeasible due to production-cost or-time, or availability of raw materials. In this work, we investigate the impact of very small data sets (<25 samples) on model quality and show how even for these data sets high quality models can be constructed.

Machine Learning in small data sets

Due to the success of Machine Learning within the context of large data sets, there is a natural interest to apply these methods in the context of small data sets and also reap their rewards here. The use of artificial intelligence and Machine Learning is these cases is generally aimed at improved design of experiments for materials optimisation, often in combination with robotic automation. Within this context the active learning approach comes naturally,[1] as it starts from a small data (sub)set, which is incrementally increased through the addition of the most useful data points in the master data set. Within the context of design of experiments, this would be newly created samples. Alternately, several authors have focussed on (small) deep neural networks in combination with small data sets (50 to several 100 samples), showing reasonable quality models.[2] These examples show that, even in the context of small data sets,

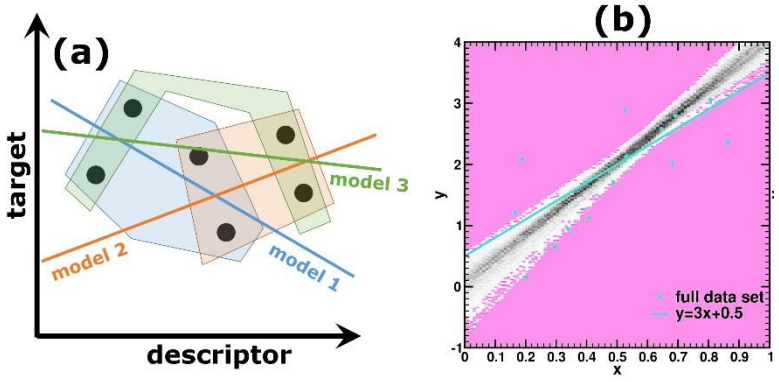

Figure 1: Modelling small data sets. (a) schematic representation of the problem. (b) and (c) heatmaps of ensembles of 1000 model instances for a linear and non-linear data set of 20 data points.[3]

Machine Learning can be successful for materials research. However, the quality of the obtained models is often defined in an ad hoc fashion and their sensitivity on the used data, though clear required human selection steps, is not discussed.

Model quality in small data sets

In this work, we present a critical investigation of the role of small (< 25 data samples) data sets in Machine Learning based regression analysis. We start from a conceptual analysis of the quality of Machine Learning models, using training, validation and test sets. In this discussion we highlight the strong dependence of the model quality on the considered data points as an important limitation of Machine Learning in this context.

Using both synthetic and experimental data sets we show that the model instances of an ensemble are distributed around the model average (cf, Fig. 1).[3,4] This result appears to be independent of the underlying model. More interestingly, we find that this ensemble average presents a model- quality on par with that of the best available model instance in the ensemble for the data set (cf, Fig. 2). We therefore propose to construct a model instance that is equivalent to the ensemble average, but presents a much lower computational cost for evaluation and storage. This mitigates the observed limitation of Machine Learning for small data sets, and makes it also accessible within the context of day-to-day small scale materials projects. [4]

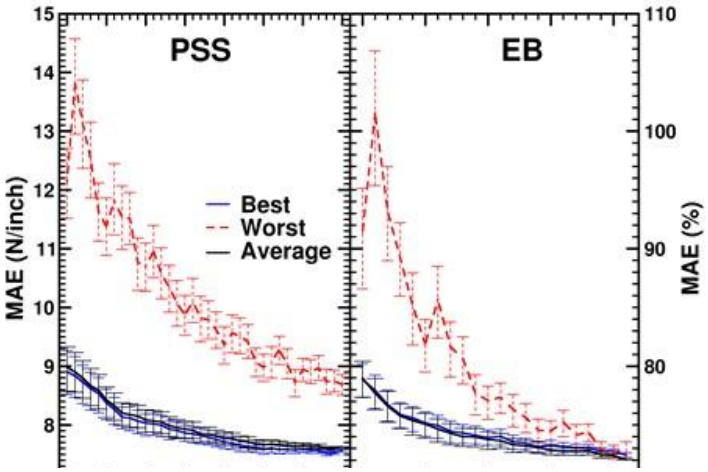

Figure 2: Estimated MAE values for the Best, Worst, and Average model instances for two experimental data sets.[3]

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Inverse atmospheric transport modelling for identifying Nuclear-Test-Ban Treaty violations

Pietter De Meutter
Belgian Nuclear Research Centre (SCK CEN), Mol

Pietter.de.meutter@sckcen.be

Abstract

Upon its entry into force, the Comprehensive Nuclear-Test-Ban Treaty will prohibit nuclear explosions by anyone, anywhere. A network of very sensitive detectors is being set up that can measure airborne trace concentrations of specific radioactive aerosols and gases that can be the signatures of a nuclear weapon test. If such radionuclides are detected, inverse atmospheric transport modelling can be used to locate the origin of the radionuclides, which helps to determine whether a Treaty violation occurred. To strengthen Treaty verification, an inverse modelling tool ("FREAR") was developed [1,2], which will be presented here together with some examples.

Smoking gun
The most recent nuclear weapon tests were conducted underground. Such underground tests are particularly challenging to detect, since radionuclides produced during and after the nuclear explosion are contained underground. A fraction of radionuclides might seep through the ground and leak into the atmosphere. Radioactive noble gases are most likely to escape underground containment. If the radionuclides enter into the atmosphere, they are transported and diluted by the wind. Upon reaching a monitoring station, the plume of radionuclides can be diluted so that only trace concentrations are present. To cope with such very low concentrations, a monitoring station samples a high volume of air through filters at a rate of 800 m^3/h. Indeed, measuring such radionuclides is crucial to discriminate a nuclear weapon test from a conventional explosion. If radionuclides are measured and subsequently linked with the seismic signals of an underground explosion event, it serves as the "smoking gun" that a Treaty violation occurred.

Optimisation problem
Atmospheric transport and dispersion models can be run backward-in-time to calculate a retroplume corresponding to an observation, which represents the area from where air sampled at the detector originated. This area increases as one goes further backward in time. Then, the retroplumes associated to all observations are coupled with a hypothetical source term (typically a point source where radionuclides were released during a specific period). The purpose is now to find such a source term that can best reconstruct the observed activity concentrations, which can be solved using optimisation techniques.

FREAR tool
An optimisation tool was developed that features two independent optimisation methods for finding source parameters such as release location, release amount and release period: (i) a cost function optimisation giving the best solution, and (ii) a Bayesian inference optimisation giving a full posterior probability distribution. The tool featuresthe ability to digest both detections and instrumental non-detections, since the latter can be used to exclude certain geotemporal source regions. The combined use of the cost function approach and the Bayesian approach offers a robust way of identifying Treaty violations if sufficient detections are available. The FREAR tool can be used not only for Treaty verification but can also in case of a nuclear accident [1,2], as it can be used to determine or refine the source term of radionuclides. In the past, it has also been used to determine the amount of Cs-137 released during resuspension from the recent wildfires in the Chernobyl Exclusion Zone in April 2020 [3], demonstrating FREAR's flexibility in its source parameterization.

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Transparent for humans, visible for birds: UV-reflecting coating for bird-safe window

Sébastien R. Mouchet[1,2], Rémy Wauters[1], Emile Haye[1], Stéphane Lucas[1] and Olivier Deparis[1]
[1] University of Namur, Namur
[2] University of Exeter, Exeter, United Kingdom

sebastien.mouchet@unamur.be

Abstract

Every year, billions of birds collide with windows, often resulting in their death, as well as in significant material damage. Some manufacturers developed UV-reflective coatings for bird-safe glazing. These coatings are often visible to the human eye over a wide range of viewing angles. In addition, the bird perception of these glazings is usually not considered in depth when developing such selectively reflective devices. However, many animal species, including birds and insects, have developed a wide variety of photonic structures active in the UV due to their perception of light in this range of the electromagnetic spectrum [1]. These structures, optimised during evolution by natural selection, allow us to elaborate new concepts of optimised coatings for selective reflection in the UV and to develop bird-safe glazing through a bioinspiration approach. We developed a bird-safe coating for flat glass panels and polymers that exploits the difference of light perception between humans and birds [2]. This coating consists of a periodic multilayer of metal oxide layers deposited on soda-lime glass substrates by Physical Vapour Deposition (PVD) with patterns. The optical response of the multilayer was numerically designed in terms of morphology and material composition, through a multi-objective optimisation, using human and avian colour perception models. Such a coating deposited on a window makes the window bird-safe, while preserving the aesthetics of the window. The deposited pattern is invisible to human eyes but strongly reflects in the UV range.

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Planetary states of the Sr atom

Matthieu Génévriez[1], C. Rosen[2], U. Eichmann[2]
[1]UCLouvain, Louvain-La-Neuve
[2] Max Born Institute, Berlin, Germany

matthieu.genevriez@uclouvain.be

Abstract

Electronic states in which two electrons are highly excited offer the possibility to study in great details correlated electron dynamics and the three-body quantum-mechanical problem. In a combined experimental and theoretical study we investigated the planetary states of the Sr atom, in which strong correlations in the two-electron motion lead to dynamics ressembling the one of planets in a solar system. These correlations also lead to unexpected effects such as strong dipole-forbidden excitation.
High lying doubly excited states are ideal to investigate the correlated dynamics of two electrons in a region where the electron repulsion and the Coulomb attraction of the ionic core have comparable magnitudes. The correlated motion cannot be explained in terms of the motion of two independent electrons, i.e. the independent-electron approximation breaks down, which leads to complex dynamics that can resemble those of two planets orbiting a star. Quasi-two-electron atoms, such as the Strontium atom, are convenient to study these effects from a theoretical and experimental point of view. The two-electron dynamics can be calculated from first principles using the method of configuration inter- action with exterior complex scaling [1]. Experimentally, high lying doubly excited states can be efficiently populated using the technique of isolated core excitation (ICE) [2], in which the two valence electrons are photoexcited to high lying orbitals in a sequential manner. Such a scheme allows one to excite the planetary states of the Sr atom [3] and can also be used for trapping [4] and quantum nondemolition detection [5] of Rydberg atoms.
We experimentally and theoretically studied the photoexcitation spectra from Sr(*5d5/2nl*) states of Sr ($n \geq 11$, $l = 9$ - *12*), located high in energy in the Sr+ continuum, to en- ergy regions close the Sr+(*5 f), Sr+(5g), Sr+(7d) and Sr+(8p*) ionization thresholds. The measured and calculated spectra are in good quantitative agreement and their complex structures, which consists of many lines and intricate intensity distributions, bear the sig- nature of large electron correlations. In the region of the Sr+(*5 f*) and Sr+(*5g*) ioniza- tion thresholds, doubly-excited states are populated by nondipole excitation. The spectra reveal the competition between electrostatic electron-electron interactions and unexpect- edly strong electric-quadrupole excitation. In the region of the Sr+(*7d*) and Sr+(*8p*) ion- ization thresholds, electron-electron interactions are even more prominent and lead to the formation of planetary sates. The two-electron probability densities show large angular correlations and confirm quantitatively the predictions of the frozen-planet approximation describing electron dynamics as the polarization of the fast inner electron by the electric field of the outer "frozen" electron.

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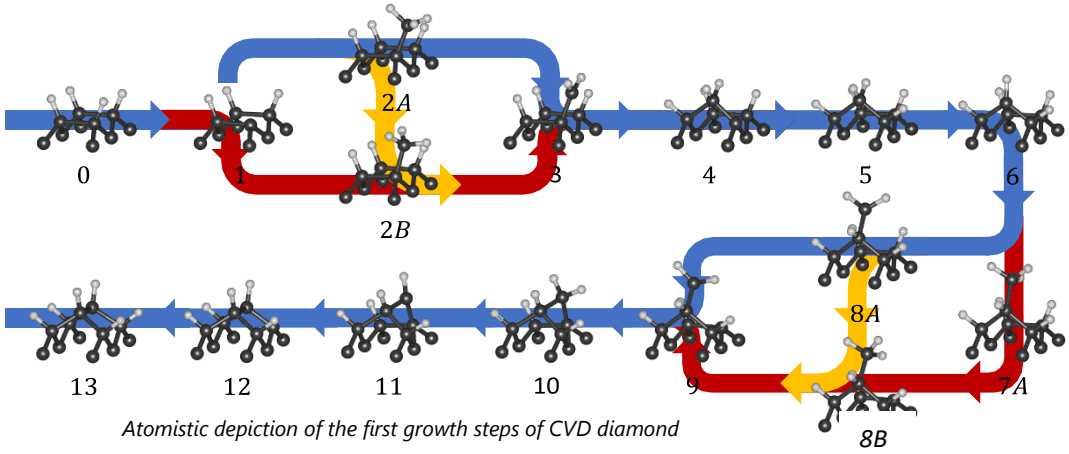
Growth mechanisms of CVD diamond

Emerick Guillaume[1, 2, 3], E. P. Vanpoucke[1, 4], L. Henrard[3] and K. Haenen[1, 2]
[1] University of Hasselt, Hasselt
[2] IMOMEC, Hasselt
[3] University of Namur, Namur
[4] Ghent University, Ghent

emerick.guillaume@uhasselt.be

Abstract

The general framework of our ongoing project is focused on the growth of the allotropic forms of carbon, ranging from sp2 (graphene) to sp3 (diamond). Despite pure diamond and graphene not being suitable for electronic applications, their doped counterparts might be tomorrow's building blocks for electronic and quantum applications. Hence the need to better understand the atomic-scale mechanisms that enhance growth rate and doping concentration of such promising materials.



Atomistic depiction of the first growth steps of CVD diamond

This work aims at calculating energy barriers among different diamond surface configu- rations to deepen our knowledge of the earliest step of diamond growth. To that end we used the Density Functional Theory and the climbing Nudged Elastic Band method [1] to determine these energy barriers of successive transitions that finally exhibit a seed, which allows for additional layer growth. Results tend to confirm published mechanisms [2, 3], but refine the height of the energy barriers previously known.

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SCK CEN Academy's STEM initiatives and perception study on nuclear science and technology

Lisanne Van Puyvelde, Michèle Coeck, Tom Clarijs and Niels Belmans
Belgian Nuclear Research Centre (SCK CEN), Mol

Lisanne.van.puyvelde@sckcen.be

Abstract

The Belgian Nuclear Research Centre SCK CEN is one of the largest research centres in Belgium with 70 years of experience in nuclear science and technology. Preserving and extending nuclear knowledge and maintaining a competent workforce in industry, healthcare, research and policy organisations are key tasks. Through its Academy for Nuclear Science and Technology, SCK CEN provides education and training at national and international level, and promotes STEM.

The SCK CEN Academy interacts with pupils and their teachers to inform them about the scientific basis and technological applications of ionising radiation. In addition specific attention is given to the pluralistic societal aspects of nuclear applications.
Amongst the various outreach activities of SCK CEN, which will be presented in this talk, the contribution to Tabloo Expoo is the most recent and comprehensive achievement. At Tabloo high school pupils, teachers, as well as the general public, discover the origin of radioactivity, the management of radioactive waste and the ongoing research in all areas and application domains. In Expoo2 the innovative experiments, the unique nuclear infrastructure, and the broad scope of the SCK CEN research activities for which the integration of multiple STEM disciplines is required, is highlighted. As such, Tabloo is an alternative for the school visits we hosted in the past on the technical domain of SCK CEN, allowing more students to get acquainted with SCK CEN's research activities.

To understand the effect of a school visit to a scientific site such as SCK CEN on the knowledge and perception of pupils towards nuclear science, applications and research, we kicked off in 2018 on an impact study. Besides general knowledge on the nuclear theme, risk estimate concerning own health in various areas, perception of nuclear, general perception of science and technology and study choice were the domains surveyed in this study. More than 250 pupils filled out a questionnaire before their visit to SCK CEN. We repeated the inquiry at two points in time after the visit. This study showed that initiatives to inform pupils in an objective way on nuclear technology are and remain indispensable.
The SCK CEN Academy aims, in collaboration with Tabloo, to continue and broaden this study in order to optimize our STEM actions.

Artificial Intelligence for materials industry: an open online course

M. Sluydts[1, 2], J. Jaeken[2]
[1] ePotentia, Deurne
[2] Ghent University, Ghent

michael.sluydts@epotentia.com

Abstract

AI4MI is an online course aiming to bridge the gap between materials researchers and artificial intelligence. It is built around four case studies which guide the user through solving practical materials problems using AI. Each case study explains the problem, the theoretical details of the models and how to use them, as well as interpretation using explainable AI. In this way it aims to increase the adaption of AI techniques for those used to working with physical models, as well as provide inspiration for researchers and educational users to include these generic AI techniques in their own projects.

Introduction

When modelling new materials we are faced with an ever-increasing amount of data during all stages of the design process. Incorporating this data in physical models can often be difficult as large amounts of data can become compute-intensive and an overabundance of parameters can make a model difficult to interpret. Moreover, a physical model requires a direct link with the material properties one wishes to describe, requiring full knowledge over the physical effects in play in the process. Modern methods in artificial intelligence provide a valuable supplement, allowing one to build models out of vast amounts of data where important parameters are automatically selected. While standard AI methods often lose interpretability, new methods in explainable AI are able to recover much of this information, providing valuable insights.

Contents

We present Artificial Intelligence for Materials industry, an open online course aimed to bridge the gap between practical materials research and artificial intelligence. The course is built around four case studies which conceptually walk you through the process of building AI models with a materials perspective.

- Case study 1 + 2 - Defects on steel plates: six classes of defects on steel plates are studied through surface images. The first case study aims to classify these images through tabular data, where important image features are extracted into spreadsheet form and used to build classical machine learning models (decision trees). The second case study aims to skip this process by using deep learning to automatically extract important image features. In both cases classification metrics are discussed in detail.
- Case study 3 - Glass screening: a dataset of refractive indices in function of glass composition is used to illustrate a screening problem. Gaussian processes are introduced as a way to build models providing measures of uncertainty which can be used to set up an intelligent sampling procedure. The optimal tradeoff between exploring the search space and exploiting the obtained results is handled by defining an acquisition function suggesting the next best candidates.
- Case study 4 – Sensor data: Various sensor data obtained from a hydraulic testing rig are used as an example set, including temperatures, pressures and cooling efficiencies. Dimensionality reduction algorithms are used to compress the time- dependent sensors to a two-dimensional space. The space is then examined for structure, showing parts of the space can be directly associated with the quality of the machine's components, enabling its usage for predictive maintenance.

We present Artificial Intelligence for Materials industry, an open online course aimed to bridge the gap between practical materials research and artificial intelligence. The course is built around four case studies which conceptually walk you through the process of building AI models with a materials perspective. Two case studies focus on detecting defects on steel plates, one on accelerating compositional screening and the final one on simplifying sensor data. While we focus on these specific applications, the same techniques can be applied on many other R&D and industrial applications and provide ideal case studies to start from for new educational material. More information can be found on https://ai4mi.epotentia.com and a free practical session will soon be organized together with the Flemish Supercomputer Center.

Educational sidenotes

The course provided a challenge since both materials researchers and AI users had to be able to understand the course. To facilitate this various choices were made. First of all the usage of in-depth mathematics was avoided where practically possible, yet theory is still treated at a deep level. As theory can still become intimidating, separate videos were made with a basic introduction and more in-depth discussions. Outside of the case studies an additional module was mode for users more focused on project management. Within the case study modules special care was taken to include also the practical pitfalls, as often AI theory comes readily implemented but quality of models are greatly affect by choices in specific parameters or through data mismanagement. Each module walks the user through the case study starting from a practical introduction of the problem, a discussion of the data (type, possible pitfalls), the typical models to handle this data, how to practically train a model on it and finally how to use explainable AI to regain materials insights. Explainable AI was chosen as an important topic to increase the confidence in AI methods, where a black box model of questionable performance can quickly violate the confidence of researchers focused on physical modelling. From the educational perspective we also took into account the form of the course. Each video was limited to +- 10 minutes, interactive questions were added in sections handling different concepts. The software Colour Simulations was used to do quality control for colorblind users and subtitles were added to ensure accessibility.

Acknowledgements

The AI4MI project was funded by the European Social Fund, the Flemish co-financing fund, OCAS and Research Foundation Flanders. The project was produced as a cooperation between ePotentia, Ghent University and OCAS NV, with input from Umicore NV and Agfa NV. More information can be found on https://ai4mi.epotentia.com and a free practical session will soon be organized together with the Flemish Supercomputer Center.

Online learning that is worth it in a post-pandemic world (efficient, flexible, social, cheap)

Stefaan Cottenier
Ghent University, Ghent

stefaan.cottenier@ugent.be

Abstract

I had been teaching a rather specialized science course in a traditional classroom setting for many years. It was well-received by about 10 students each year at my university. At some point I realized I was using a learning format optimized for 15th century technology (classrooms, books). Can my students gain something if I were to use 21st century technology instead (internet, videos, connectivity)? And am I able to make this change, as a single teacher without a budget? In this presentation, I will use my course as an example to answer these questions.

Emphasis will not be on my course as such, but on the general reasons why this approach turned out be successful. And on the prerequisites and boundary conditions that matter for you to be able to copy parts of this format.

I will also show how this course is now being adopted at other universities, and how volunteering learners from around the globe use it. The yearly audience has grown from 10 to +100: I feel much more useful now, while it doesn't take me more time than before. I will argue that this course format is low-hanging fruit for sharing courses among universities.

My conference talks on Youtube: http://bit.ly/cottenier

Poster presentations

List of posters

Author	Affiliation	Title
Lorena Ballesteros Ferraz	UNamur	Tackling quantum algorithms using modular values
Marie Bernardi	UMons	Study of Cr(III) and Mn(II) loaded resin by benchtop nuclear magnetic resonance
Eduardo Marin Bujedo	UCL	Autoionization rates of core-excited Rydberg states of Sr
Vana Chinnappa Chinnabathini	KULeuven	Composition-tuned Au-Ag bimetallic clusters-modified TiO2 films as efficient self-cleaning surfaces under visible light
Evelyne Daubie	UMons	Possibility of making semiconductor-based sensors autonomous in energy by means of energy harvesting in a nuclear environment
Sarah Doumen	UHasselt	Physics for a sustainale future: the case of the new Master of Materiomics
Yves Gossuin	UMons	Characterization of commercial iron oxide clusters as potential Magnetic Resonance Imaging contrast agents
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Serghei Klimin	UAntwerpen	Collective excitations of a charged Fermi superfluid in the BCS-BEC crossover
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Fiona Crystal Mascarenhas	IMEC	Lab-scale HAXPES - new tool enabling the study of buried layers and interfaces
Đorđe Petrović	SCK CEN	Investigation of a hypothetical core disruptive accident in Multipurpose hYbrid Research Reactor for High-tech Applications (MYRRHA))
Thanh Trung Pham	UNamur	Graphene on Si(111) 7x7
Steve Smeets	UMons	Photonic modeling of two-photon spontaneous emission processes beyond the electric dipole approximation

Tackling quantum algorithms using modular values 2022 Annual Meeting of the Belgian Physical Society

Lorena Ballesteros Ferraz[1], Timoteo Carletti[2] and Yves Caudano[1]
[1] University of Namur, Namur
[2] University of Namur, Namur

lorena.ballesteros@unamur.com

Abstract

Quantum algorithms can solve problems more efficiently than classical ones. Among the first and most representative examples of this superiority are the Deutsch algorithm and its generalization, the Deutsch-Jozsa algorithm. The latter verifies if a function, $f : \{0, 1\}^N \longrightarrow \{0, 1\}$, is balanced or constant. The quantum procedure only needs one step to solve the problem while the classical one requires 2^N -1 repetitions in the worst case.
Usually, measurements are considered ideal, non-reversable projective operations. To perform one, the system should interact with a measuring device, or ancilla. For some measurements, the system and the ancilla interact through a unitary operator. In that case, when the interaction strength between the system and the measuring device is weak enough, the unitary operator can be expanded in a Taylor series to first order. This consti- tutes a weak measurement. When describing the observations of quantum weak measure- ment with pre-selection (which consists of choosing the initial state) and post-selection (which requires a projective measurement after the weak measurement and corresponds to choosing the final state), quantities called weak values appear. In that case, the ancilla's wavefunction is shifted in position by an amount that is proportional to the real part of the weak value. Its wavefunction is also shifted in momentum by an amount that is pro- portional to the imaginary part of the weak value. As the weak value is an unbounded and complex number, it has found several applications in metrology, sensing, as well as in quantum foundations and probing quantum paradoxes.
When considering observables that are unitary, the modular value, $A_m = \frac{\langle \psi_f | e^{-ikA} | \psi_f \rangle}{\langle \psi_f | \psi_i \rangle}$,
arises. It is linked to the weak value in very specific cases, in between others, when k is small and the exponential can be expanded in Taylor. Nonetheless, modular values are associated to an interaction of any strength, a weak coupling between the system and the ancilla is not needed.

In this work, we present a new approach to quantum algorithms using modular values. The procedure exploits the degrees of freedom and complex properties of modular val- ues. It could reduce the involved number of gates and hence the error in the execution of the algorithm. Nonetheless, the method always requires one extra qubit to readout the result of the quantum modular value.
We applied this procedure to the Jozsa and Deutsch-Jozsa algorithms both theoretically and experimentally, in the IBM Quantum Computer.

Study of Cr(III) and Mn(II) loaded resin by benchtop nuclear magnetic resonance

M. Bernardi, .L. Hantson and Y. Gossuin
University of Mons, Mons

marie.bernardi@umons.ac.be

Abstract

Heavy metals ions such as Cr(III) and Mn(II) are known to be toxic and must be removed from wastewater. These ions have also paramagnetic properties which allowed the use of Nuclear Magnetic Resonance (NMR) relaxometry to monitor their removal from water by a strong cation exchange resin. In this research, kinetic and equilibrium isotherm experiments were performed.

Heavy metals have become a major public health and environmental concern [1]. The removal of these metals from water is often performed by ion exchange. In this context, ICP-AES spectroscopy is currently used to study ion exchange efficiency. However, this technique is indirect and destructive. Some heavy metal ions like Cr(III) and Mn(II) have paramagnetic properties that can affect the Nuclear Magnetic Resonance (NMR) relaxation times T_1 and T_2 of water protons which can be easily measured by benchtop NMR relaxometry [2-3]. Therefore, T_1 and T_2 can be used to follow the evolution of the concentration of paramagnetic ions in solution and thereby monitor the removal of heavy metals by a strong cation exchange resin.
Batch experiments were carried out to study the ion exchange kinetics: a sample containing a small amount of Dowex Marathon MSC resin was put in contact with aqueous solutions containing the paramagnetic ion of interest before being shaken by a vortex mixer (Figure 1). The transverse relaxation time (T_2) was measured at different time intervals which allowed the monitoring of the amount of adsorbed metal. Repeating the same experiment with different metal concentrations provided the adsorption isotherms.
The experimental kinetic data were in good agreement with the pseudo-first order kinetic model. The equilibrium isotherms of Cr(III) and Mn(II) were described by the Langmuir and Freundlich models.
The next step will be to reproduce these experiments with other adsorbents like activated carbon at different magnetic fields. In the future, it will also be interesting to carry out a so-called NMR column experiment in order to follow the loading of resin in real-time through the measurement of the NMR signal.

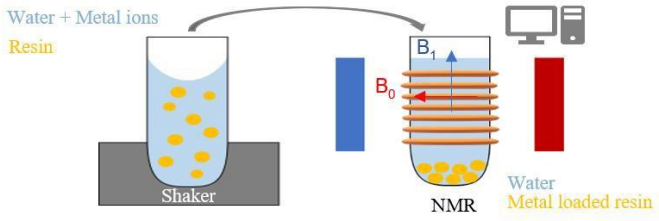

Figure 1. Experimental set-up

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Autoionization rates of core-excited Rydberg states of Sr

E. Marin-Bujedo, M. Génévriez
UCLouvain, Louvain-la-Neuve

eduardo.marinbujedo@uclouvain.be

Abstract

Atoms in core-excited Rydberg states lie above the first ionization threshold and can decay spontaneously by emitting one electron in a process called autoionization. Although it is well known that the autoionization rates scale with the principal quantum number n of the Rydberg electron as $1/n^3$, their evolution with the angular-momentum quantum number ℓ is poorly known. We have performed theoretical calculations to determine the autoionization rates of core-excited Rydberg states in Sr atoms for a broad range of values of ℓ to characterize their behavior.

Atoms and molecules in a core-excited Rydberg state possess one electron excited to a high-lying orbital whereas the residual ion core is in a low-lying excited state. These states lie energetically over the first ionization threshold and can decay rapidly by autoion- ization. It is well known that the autoionization rates decrease with the principal quantum number n of the Rydberg electron as $1/n^3$. Their scaling with the Rydberg-electron orbital-angular-momentum quantum number ℓ, on the other hand, is still unknown [1, 2]. We present a theoretical study of the autoionization rates of the core-excited Rydberg
states of Sr atoms for a fixed value of n = 45 and a broad range of ℓ values. Sr atoms, like any other alkaline-earth-metal atom, possess only two valence electrons, which makes extensive and accurate calculations feasible. Core-excited Rydberg states combined with cold atomic gases have promising applications in the fields of quantum simulation and quantum information processing [2, 3], for which a detailed knowledge of the autoionization rates is required. A better understanding of the ℓ-dependence of the autoionization rates is also important to estimate more accurately the autoionization lifetimes of Stark-mixed Rydberg states, such as the ones used for pulsed-field-ionization zero- kinetic-energy photoelectron spectroscopy, as well as dielectronic recombination rates. We performed large-scale calculations of the autoionization rates of Sr using the method of configuration interaction with exterior complex scaling (CI-ECS) [4]. CI-ECS allows the treatment of the two-valence-electron dynamics in its full dimensionality and does not rely on the assumptions made in other widely used methods [4]. Diagonalization of the complex-scaled Hamiltonian calculated using numerical basis functions directly provides the autoionization rates of the core-excited Rydberg states. Our first results agree with the rapid decrease of the autoionization rates with ℓ observed in other studies (see, e.g., Refs. [1, 2]) and a detailed characterization of this behavior with respect to all relevant angular-momentum quantum numbers is under way.

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Composition-tuned AuAg bimetallic clusters-modified TiO2 films as efficient self-cleaning surfaces under visible light

Vana Chinnappa. Chinnabathini[1] , Fons Dingenen[2], Rituraj Bora[2], Didier Grandjean[1], Sammy W. Verbruggen[2] and Ewald Janssens[1]
[1] KU Leuven, Leuven
[2] University of Antwerp, Antwerp

chinnabathini.vanachinnappa@kuleuven.be

Abstract

Surface modification of titanium dioxide photocatalysts with plasmonic metal nanoparticles is a promising way to extend the operation window to the visible light region, corresponding to the maximum output range of the sun's total irradiance spectrum.[1] These photocatalysts are tested for the degradation of stearic acid (SA) since it is a widely applied method for assessing the photocatalytic activity of self-cleaning materials. SA is a good model compound for organic fouling on glass windows.[2]

We studied the stearic acid degradation on TiO2 decorated with 1.5-2.5 nm AuAg bimetallic clusters of different compositions both under UV and simulated solar light. Mono- and bimetallic Au_xAg_{1-x} (x=0, 0.1, 0.3, 0.5, 0.7, 0.9 and 1) clusters produced in a noble gas environment were soft-landed using cluster beam deposition (CBD) on TiO_2 P25-coated silicon wafers with a coverage of 4 atomic monolayer equivalents. While the photoactivity of the obtained films towards stearic acid degradation compared to pristine TiO_2 is basically unchanged under UV, a significant enhancement is observed under solar simulator with a very clear composition-dependent volcano-type trend peaking at the $Au_{0.7}Ag_{0.3}$ composition. This behaviour may originate from their composition-dependent atomic arrangements and electronic structures stemming from their nucleation mechanism.[3,4]

These results demonstrate the excellent potential of the CBD technology to fabricate novel and efficient noble metal modified photocatalytic surfaces with a high control over cluster size, coverage, and composition, without involving potentially hazardous chemical agents.

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Possibility of making semiconductor-based sensors autonomous in energy by means of energy harvesting in a nuclear environment

A.Quenon, E. Daubie, F. Dualibe and V. Moeyaert
University of Mons, Mons

evelyne.daubie@umons.ac.be

Abstract

One way to ensure the long-term operation of an electronic device is to power it by using ambient energy harvesting. Different forms of energy harvesting methods are known and already exploited in equipment, such as photovoltaic panels, thermoelectric generators, or radio-frequency antennas. The principle is to generate electrical power by converting the solar, mechanical or electromagnetic energy into direct current electricity.

We propose energy harvesting based on the use of ionization trails produced by a high flux of ionizing radiation as it passes through a sensitive material. More precisely, the objective is to harvest the ionization current produced by the primary electron-hole pairs moving under the "diffusion" electric field present at a pn junction.

We present the results of the tests carried out in order to prove the validity of our idea [1]. We describe the experimental setup that we have built, in particular the 3D printed mechanical system designed to control the location of the radioactive source in front of the semiconductor device under test. The tests are based on real-time characterization of the electrical response of the irradiated device. For that, open-source software [2] was written permitting a remote control of the measurement instrument [3]. Our investigations show that commercial photodiodes generate a few pA dc, enough to power integrated analog blocks.

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Physics for a sustainable future: the case of the new Master of Materiomics

S. Doumen, J. Notermans, K. Denolf, D.E.P. Vanpoucke and An Hardy
University of Hasselt, Hasselt

Sarah.doumen@uhasselt.be

Abstract

In 2022-2023, the new Master of Materiomics starts at UHasselt. This program is aimed at students who want to develop sustainable, innovative materials at the interface of physics and chemistry and on the basis of both theoretical/computational and experimental approaches. There are 4 specialization areas: materials for quantum technologies; innovative healthcare; circular processes; and energy. The combination of viewpoints and the boundary crossing nature of the program prepares students for the interdisciplinary teams of the future. As interdisciplinary physics experts, these students will tackle material-related issues in response to societal grand challenges such as climate change and energy transition.

Breakthrough materials development for a sustainable future

At this very moment, society faces complex and intertwined grand challenges, e.g., climate change, pandemics, innovative and safe communication technologies, the energy transition, changing industrial processes, innovative space research and finite resources that are becoming depleted. In response to these challenges, there is a high demand for scientists who are ready for an internationally-oriented and interdisciplinary research environment and labour market. One of the core fields in this respect is materials development and research, as some solutions to the above mentioned complex societal issues may lie in the development of new technologies, of which breakthrough materials development is an important component. Within this context, in 2022-2023, the new Master of Materiomics starts at UHasselt, aimed at students who want to develop alternative, sustainable materials which may help society to remain within planetary boundaries and not to overshoot. To focus the program 4 possible core areas of specialization are defined: Quantum, Energy, Circularity and Health. Flemish students who obtained an academic bachelor in physics have direct access to the master's program, next to academic bachelors in chemistry, biochemistry and biotechnology, bioscience engineering, and engineering sciences. The goal of the master's program Materiomics, is to train interdisciplinary T-shaped professionals, i.e., experts in their field (e.g., physics) who are able to build bridges between the different perspectives involved in materials research and development (cf, Fig. 1). The term 'Materiomics' refers to the holistic study of processes, structures and properties of materials from an exact scientific fundamental, systematic perspective through all relevant scales, from atomic to macroscopic, into the synthesis and functionality. Masters of Materiomics have a solid, broad knowledge base in which the modeling, design, synthesis, properties, and characterization of materials play a central role. Materials are studied from an interdisciplinary perspective, building bridges not only between physics and chemistry, but also between experimental and theoretical methods: Students are taught to

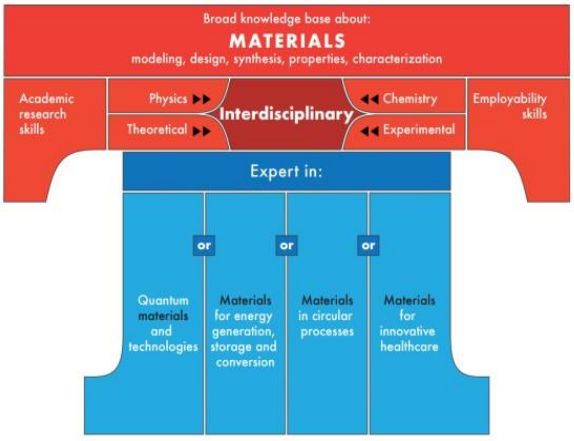

Figure 1: The profile of the Master of Materiomics as an interdisciplinary T-shaped professional.

approach materials from different perspectives and learn to communicate across disciplinary boundaries with experts in chemistry etc., with due attention to academic research skills and soft skills which prepare them for their professional careers. In addition to a broad knowledge base, students acquire in-depth knowledge and skills in one of the 4 areas of specialization: quantum materials and technologies (with applications in cyber security, satellites, medical diagnostics, etc.), materials for energy generation, storage and conversion (from flexible solar cells, over thermochromic glazing to sustainable battery materials), for circular processes, or for innovative healthcare.

Training interdisciplinary physics experts

To obtain these goals, interdisciplinary competences are required: students need to cross boundaries between physics and chemistry, as well as between experimental and theoretical/computational methods. Interdisciplinarity is gradually introduced throughout the curriculum, building on the four learning mechanisms from boundary crossing theory [1, 2], i.e. identification, coordination, reflection and transformation (cf, Fig. 2). More specifically, students are introduced to the different perspectives and approaches, to making connections between different perspectives, synthesizing them (e.g. through assignments, group work...), and applying all this to new, complex material problems (e.g. through a hands-on project, the internship and master's thesis).

Figure 2: The four learning mechanisms of boundary crossing theory [1, 2].

In this lecture, some examples will be presented of how these learning mechanisms can be addressed in different courses and their teaching and assessment approaches [3, 4], to ultimately train experts in physics capable of addressing complex material issues from a holistic approach in multi- and interdisciplinary teams with the necessary attention for aspects such as sustainability, availability of raw materials, recyclability and cost.

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Characterization of commercial iron oxide clusters as potential Magnetic Resonance Imaging contrast agents

Y. Gossuin, E. Martin, Q. L. Vuong, J. Delroisse, Sophie Lauren, Dimitri Stanick, Cédric Roussea
University of Mons, Mons

yves.gossuin@umons.ac.be

Abstract

The physicochemical, magnetic and Nuclear Magnetic Resonance (NMR) relaxation properties of clusters of iron oxide particles are studied. The results show that these clusters, initially intended for magnetofection, are excellent candidates as contrast agents for Magnetic Resonance Imaging (MRI).

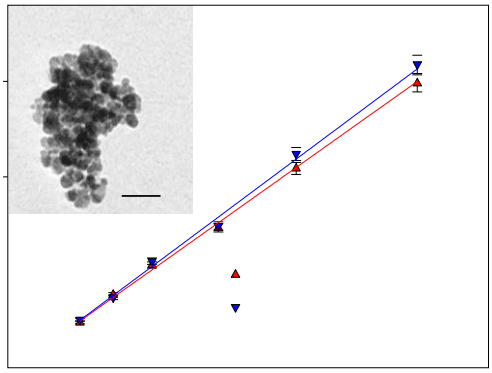
Introduction

Superparamagnetic iron oxide particles (SPIOs) have been used for 20 years as contrast agents for clinical Magnetic Resonance Imaging (MRI) [1] and are still intensively used for molecular and cellular imaging in preclinical studies on small animals [2]. For the latter application, clusters of iron oxide cores are especially efficient because their effect on the transverse NMR relaxation time (T_2) can be huge – far larger than what can be achieved with usual gadolinium contrast agents. The Polymag™ iron oxide clusters have initially been developed for magnetofection – i.e. the introduction of nucleic acids inside cells using magnetic particles and a magnetic plate creating magnetic field gradients [3]. These clusters are here studied as potential contrast agents for MRI thanks to a multidisciplinary characterization including dynamic light scattering, electron microscopy, magnetometry and NMR relaxometry.

Results and discussion

The Polymag™ clusters present a hydrodynamic diameter of 180 nm with a large polydispersity index (PDI = 0.15). The image of a typical cluster, obtained by transmission electron microscopy, is shown in the inset of figure 1. The diameter of the cores constituting the clusters, determined by magnetometry, is assumed to follow a lognormal distribution with $d_{0,c}$ = 4.9 nm and σ = 0.53.

The magnetization of the cores is M_v = 371000 A/m. The transverse relaxivity of the clusters, defined as the increase of the relaxation rate $1/T_2$ for an increase of 1 mM of iron concentration, is remarkably high:
r_2 = 470 $s^{-1}mM^{-1}$ at 1.41 T and 37°C (Figure 1), which is close to the maximum achievable relaxivity of ~ 750 $s^{-1}mM^{-1}$.



[Fe] (mM)
Figure 1: evolution of $1/T_2$ of aqueous solutions of the Polymag ™ clusters with the iron concentration

The transverse relaxation is independent of temperature and of the interecho time used in the measurement sequence. From the theoretical point of view, the clusters should be mainly in the Static Dephasing Regime (SDR), which explains their large relaxivity [4]. The Polymag™ clusters are thus good candidates for cellular MRI since they can be internalized into cells using the transfection protocol. However, one disadvantage of such large clusters is their reversible clustering within the magnetic field of the NMR device, which has been proven thanks to the evolution with time of the measured T^1 and T^2.

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Inclusion of electronic correlation on optical, electronic and magnetic properties of materials.

A.Honet[1], L. Henrard[1] and V. Meunier[2]
[1] University of Namur, Namur
[2] Rensselaer Polytechnic Institute, New York, USA

Antoine.honet@unamur.be

Abstract

In general, optical properties from materials can be deduced from their electronic properties. Among electronic techniques, the most current are ab initio techniques such as Density-Functional Theory. Besides these ab initio techniques, a possible road to compute electronic properties are model Hamiltonians that are parametrized and thus (semi-)empirical. Nevertheless, the computational cost is a lot reduced from ab initio computational, rending possible to model larger nanosystems or effects that are usually set aside in ab initio computations, such as correlation.

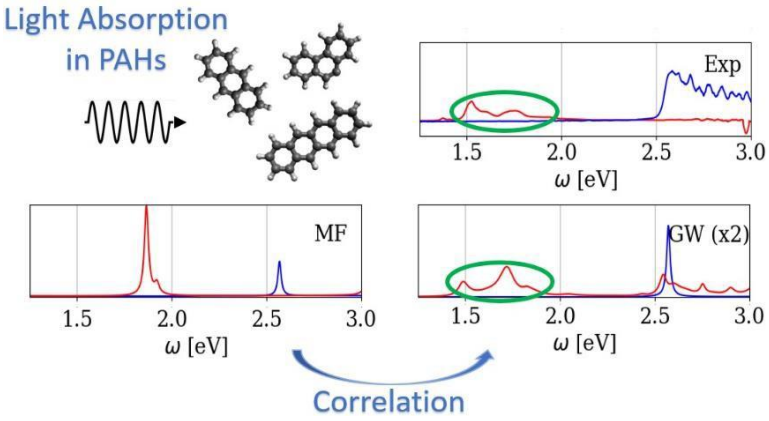

Fig. 1: Optical absorption cross section of anthracene computed in MF, GW (bottom panels) compared with experimental date (top panel). Blue curves correspond to the absorption of neutral particle whereas red curves are the absorption of the anion with one added electron. The improvement from MF to GW highlights the importance of correlation effects.

We present here a Green's functions formalism applied to model Hamiltonians that allows for computing electronical, optical and magnetic properties of nanoparticles as well as for including correlation, through the GW approximation of the Hubbard model. Optical properties of small polycyclic aromatic hydrocarbons have been investigated and compared to experiments (see Fig. 1) and fundamental effects of correlation are tackled for very small systems (see Fig. 2).

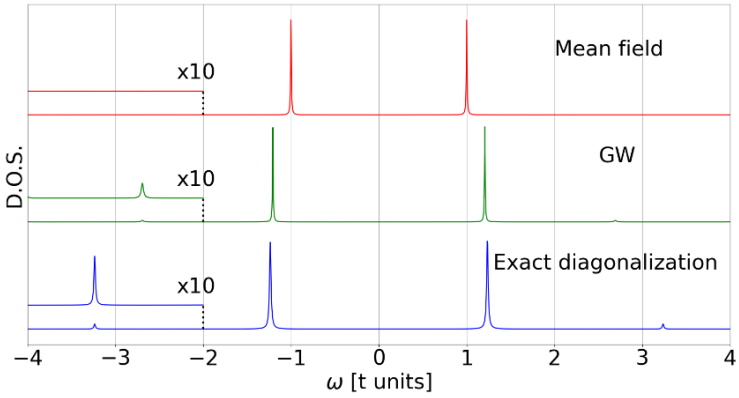

Fig. 2: Comparison of the Density of states for a two-site Hubbard model computed in the mean-field approximation, in the GW approximation and using exact diagonalization technique. The former neglects the correlation whereas the latter includes all the

correlations from the Hubbard model. The GW approximation is a step towards exact diagonalization form mean-field approximation.

Fundamental effects of correlation on electronic, optical and magnetic properties are still misunderstood and we intend correlation playing an important role in collective phenomena such as plasmons.

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Extending Feynman's variational path integral approach: Application to the Bose polaron problem

T. Ichmoukhamedov and J. Tempere
University of Antwerp, Antwerp

Timour.ichmoukhamedov@uantwerpen.be

Abstract

Nearly a century ago Landau has pioneered the solid state polaron idea [1], where an electron becomes dressed by the phonons of a crystal lattice and forms the polaron quasiparticle. Since then, similar behavior has been observed in various different physical systems [2-4], hereby broadening the polaron quasiparticle concept. Recently, the Bose polaron, where an impurity atom is immersed into a Bose-Einstein condensate has been observed in two different experiments [5,6]. Interestingly, most polaron models reduce to a similar Fröhlich Hamiltonian form [7] at weak coupling, which has been the subject of extensive theoretical study.

For many decades now, the superior semi-analytic tool of choice to study the ground state properties of various Fröhlich models has been Feynman's variational path integral approach [8] which has previously shown remarkable agreement with Monte Carlo results for the energy. However, for the Fröhlich model associated with the Bose polaron – the Bogoliubov-Fröhlich model, surprisingly large discrepancies have been found from the Monte Carlo results [9]. It has been shown that the model contains a highly subtle UV behavior that is not captured by other commonly used polaronic theories [10].

In this poster we present our results where we have combined previously proposed ideas to improve Feynman's approach [11-13] and applied them to the Bogoliubov-Fröhlich model. We find major improvements for the ground state energy in excellent agreement with Monte Carlo calculations, and retrieve the correct UV behavior of the model. In doing so we address previously existing concerns regarding applications of this approach for the Bose polaron and reaffirm the method to be a useful semi-analytic tool for various polaronic models.

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Collective excitations of a charged Fermi superfluid in the BCS-BEC crossover

S. N. Klimin[1], J. Tempere[1], H. Kurkjian[2]
[1] University of Antwerp, Antwerp
[2] Université de Toulouse, Toulouse, France

Sergei.klimin@uantwerpen.be

Abstract

We present a review of our recent studies of collective excitations in a superfluid state of condensed Fermi gases, with a particular attention to charged superfluids and superconductors. We are focused on the dispersion and damping of collective excitations at nonzero temperatures, accounting for coexistence and interaction of different branches of collective excitations: plasma oscillations, pair-breaking "Higgs" modes, and phononic-like Carlson-Goldman excitations.

Dispersion and damping of collective excitations

Collective excitations offer a possibility for sensitive experimental tests of the microscopic physics of many-body systems.

The path integral approaches for superfluid fermionic gases and for a Coulomb gas have been combined in a unified formalism, extending the Gaussian fluctuation approximation to account for plasmonic modes. This Gaussian pair-density fluctuation approach (GF) is equivalent to the random phase approximation (RPA) and is capable to describe all branches of collective excitations existing in a charged superfluid/superconductor:

- plasma oscillations
- pair-breaking "Higgs" modes
- phononic-like Carlson-Goldman excitations

The GF/RPA method describes collective excitations in the whole crossover between the weak-coupling regime of the Bardeen – Cooper – Schrieffer (BCS) pairing and the strong-coupling regime of the Bose-Einstein (BEC) condensation of molecules in real space. In the far BCS regime, we have described analytically the low-momentum quadratic dispersion of superconducting plasmons in 3D, and the resonance splitting which occurs when the eigenenergy nears the pair-breaking threshold. The present method may also be applied to a superfluid state of ultracold fermions where different kind of long-range interactions can be engineered with dipolar atoms.

Frequencies and damping factors of collective excitations in the BCS-BEC crossover can be determined in two complementary ways: (i) through spectral weight functions for the density and pair field responses; (ii) in a semi-analytic way as complex poles of the fluctuation propagator analytically continued through a branch cut. Using both methods in parallel and comparing results of them, we can reliably identify collective modes.

The case of a particular interest occurs when the plasma frequency is of the same order as the pair-breaking continuum edge. Particularly, the Carlson-Goldman mode in the BCS- BEC crossover can survive in a broader temperature range than in the far BCS limit.

In the BCS-BEC crossover, plasma and pair-breaking modes can interact with each other, because they are not, in general, purely amplitude or phase excitations. As a result, pair-breaking and plasma excitations exhibit anticrossing near the continuum edge and show an enhancement of the pair- breaking mode response at resonance.
Fig. 1 shows contour plots of spectral weights for the modulus and phase responses of the pair field at a fixed value of the momentum $q = 0.4(2m\Delta)^{1/2}$. The avoided crossing of pair-breaking and plasma branches of collective excitations is clearly seen in the spectral weight functions. Also, the modulus response exhibits a resonant enhancement due to mixing of plasma and pair-breaking modes as also predicted by analytic calculations of complex poles of the fluctuation propagator. This resonant behavior makes pair-breaking modes promising for their experimental observation.

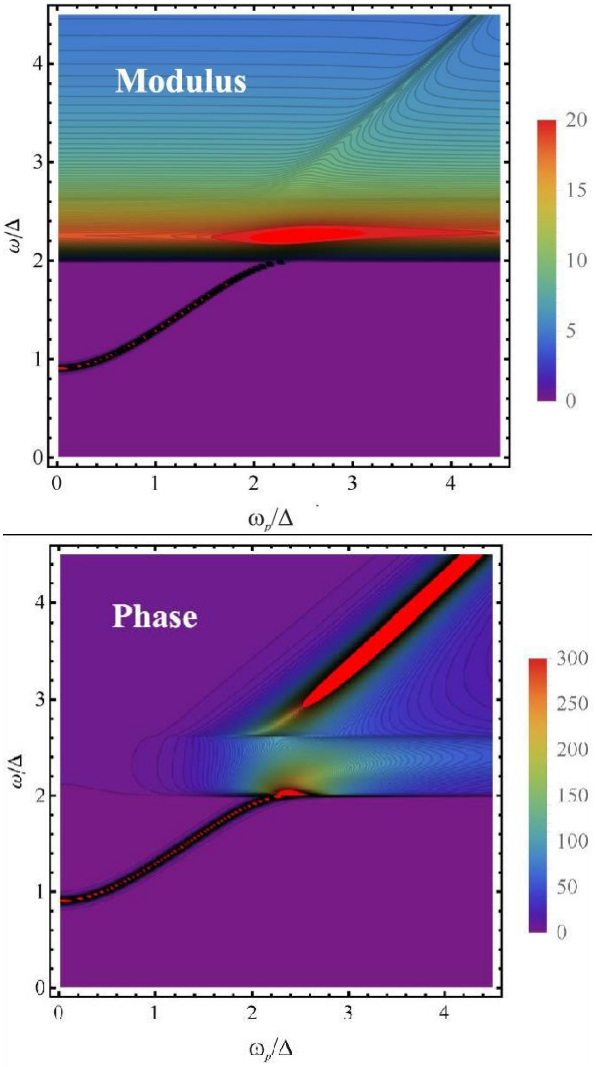

Fig. 1. Contour plots of the modulus and phase pair field spectral weight functions for a charged Fermi superfluid vs the response frequency ω and the bare plasma frequency ω_p at T = 0 in the BCS regime with the inverse scattering length (in units of the Fermi wave number k_F) $1/k_F a_S = -1$

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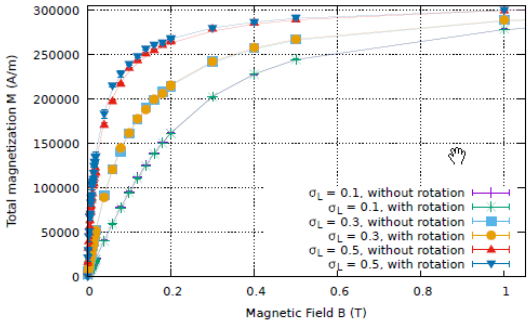
Monte Carlo and Experimental Study of the Magnetic Behaviour of Superparamagnetic Nanoparticles

E . Martin[1], Y. Gossuin[1], S. Bals [2], S. Kavak [2], Q. L. Vuong [1]
[1] University of Mons, Mons
[2] University ofAntwerp, Antwerp

Eleonore.martin@umons.ac.be

Abstract

Superparamagnetic Iron Oxide Nanoparticles (SPION) are nanosize crystals of magnetite or maghemite. Their peculiar magnetic properties makes them particularly suited for a variety of biomedical applications, ranging from cellular imaging to cancer treatment by hyperthermia [1]. The usual theory used to describe their magnetic behaviour is that de- veloped by Paul Langevin [2], which only applies to idealized (isotropic, monodisperse in size and non-interacting) nanoparticles at high temperatures. Reality however always deviates from that theoretical framework: real samples exhibit polydispersity in sizes, particles usually have at least one anisotropy axis, and, particulary in biological media, they tend to aggregate, leading to locally high particle volumic fractions and therefore interaction between their magnetic moments [3]. All those phenomena impact the mag- netization of particle ensembles in a non-trivial way and are impossible to model simul- taneously theoretically.
In this work, these deviations from the Langevin law are studied numerically, at thermo- dynamic equilibrium and at 300K, using a Metropolis algorithm, and compared with ex- perimental data obtained using a Vibrating Sample Magnetometer for real SPION, whose size distribution was evaluated by transmission electron microscopy. Thorough tests are led on the simulations to ensure convergence of the magnetization. The effect of each parameter on the field-dependent magnetization curves is then studied.
Figure 1 shows an example of the impact of one of those parameters: inhibiting rota- tion of the particles (i.e. the Brown relaxation process). As can be seen, it leads to a slower saturation of the magnetization in samples with a high size dispersion parameter
(σ_L = 0.5). Likewise, the presence of dipolar interaction between particles also leads to slower saturation in such samples, as does drying samples under a magnetic field perpen- dicular to the measurement field (as opposed to drying them under a field parallel to the measurement field, which yields the opposite effect). These various modifications of the curves result in erroneous size dispersion parameters when fitting them to an integrated Langevin equation. The simulations compare well with experimental results, as can be seen on figure 2. In future work, the simulations could be improved by changing the anisotropy model from uniaxial to a more realistic cubic anisotropy.



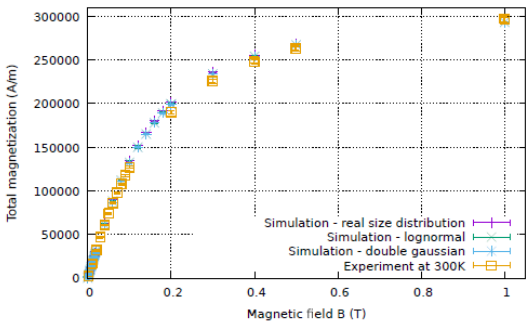


Figure 1: Impact of the particles' ability to rotate on the magnetization curve of particles with a lognormal distribution of their radii, a 3nm median radius and varying size dispersion parameters (σ_L = 0.1,0.3,0.5.

Figure 2: Comparison between experimental results (in or-ange) obtained on HiQ Nano 6nm maghemite nanoparticles, and three simulations differing in the particle size distribution.

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Lab-scale HAXPES - new tool enabling the study of buried layers and interfaces

Fiona Mascarenhas[1,2], Thierry Conard[1], Anja Vanleenhove[1], Ilse Hoflijk[1]
[1] IMEC, Leuven
[2] KU Leuven, Leuven

Fiona.Crystal.Mascarenhas@imec.be

Abstract

In this presentation, we will demonstrate the possibilities of the HAXPES lab-scale systems for application in the semiconductor industry and investigate the challenges we need to overcome. First, we describe one of the challenges while dealing with dielectrics which is Binding Energy Referencing and discuss mitigation methods. Then, we apply the learning to the chemical analysis of interfaces in multi-layer high-k/metal gate stacks and investigate the modifications of the layer chemistry of the buried layers upon thermal treatments.

Recent advances in semiconductor industry require the study of surfaces, interfaces, and buried layers especially during process development to enhance the performance of devices. Several approaches have been used to fulfil these analysis needs. One used characterization technique is photoelectron spectroscopy (PES). PES is based on the principle of the photoelectric effect, which is used to obtain physical and chemical information of materials. Traditionally, lab- based photoelectron spectrometers are equipped with soft X-rays sources (less than 2 keV) which only enables analysis of surfaces or interfaces within the top few nanometers. Deeper buried interface layers require the use of destructive profiling methods (sputtering), which can result in a strong chemical modification of the examined layers/interfaces.
A way to alleviate the depth limitation is to increase the photon energy which allows getting information on deeper interfaces and buried layers. Earlier these high energy photon sources (Hard X-rays) were confined to synchrotrons. But recently there are developments of several lab-scale instrument using predominantly Cr Kα photons (5.4 keV) [1] or Ga Kα photons (9.25 keV) [2] [3]. These two sources along with a soft X-ray Al Kα source (1.48 keV) were used in this work.

HAXPES, as new metrology tool faces several challenges. One of the main challenges is Binding Energy Referencing. Materials such as dielectrics undergo charging during the photoemission process and the presence of multiple layers of various conductivity in the stack leads to vertical differential charging. An understanding of this differential charging is critical for Binding Energy Referencing. As an example, Figure 1 and 2 show changes in binding energy position difference (between Si HAXPES peaks related to unoxidized Si and the Si HAXPES peaks related to SiO2) in simple SiO2/Si stacks when using different X-ray source energies for the measurement or when changing the SiO2 layer thickness. In this presentation we will further elaborate on the peak shifts due to charging along the depth and the variation between peak positions with different sources/photocurrent. We shall also discuss how different mounting schemes have an influence on the reproducibility of measurements. It is important to develop a protocol to overcome these challenges.
HAXPES was then applied on technologically relevant samples from the semiconductor industry and more specifically on high-k/metal gate stacks which are critical in transistor fabrication. Annealing is a critical stage during manufacturing of gate stacks and may lead to chemical modifications at interfaces. Our main goal is to characterize the chemical modification at the surface, interface and inside buried layers of gate stacks pre and post annealing. With this presentation we will show how, with the lab based HAXPES tool, we analyze the interfaces and buried layers of a multilayer stack (such as TiN/HfO2/SiO2/Si) without damaging the sample. The HAXPES spectra in Fig 3 show how the deposition of an extra layer (changes in Hf 3d spectrum upon TiN deposition) or the annealing of the full layer stack (changes to Ti 1s and W 3d spectra) results in visible changes on the HAXPES spectra.

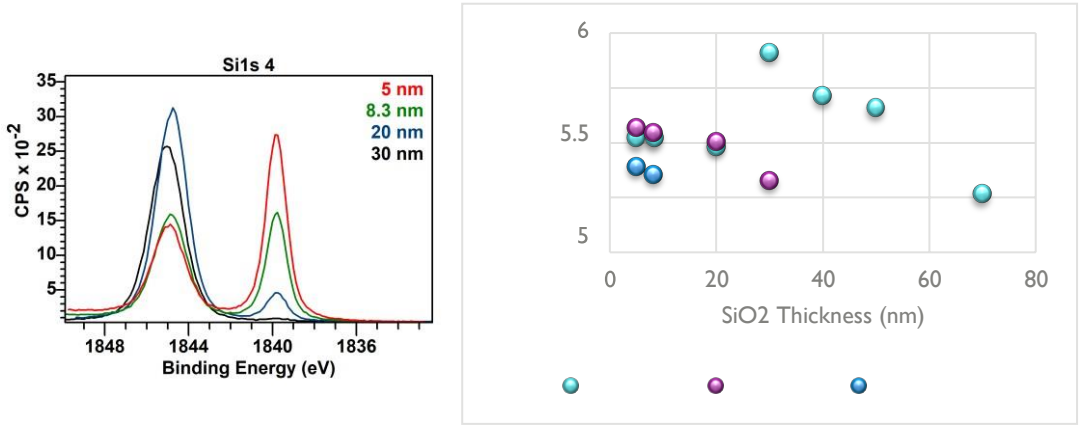

Fig. 1: Si1s spectra from SiO2 /Si substrate stacks with different SiO2 thicknesses, measured using a Cr Kα X-ray source
Fig 2- Si 1s or Si 2p Peak Energy Difference between the Si and SiO2 component of the XPS/HAXPES curves for different SiO2 layer thicknesses and different X-ray sources.

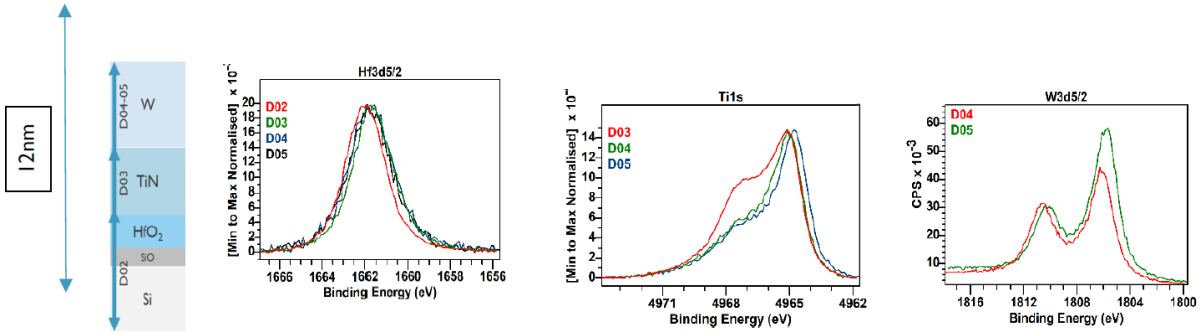

Fig 3: Comparison between the HAXPES spectra (Hf 3d, Ti 1s and W 3d(Ga Kα)) of layers in a multilayer stack pre and post annealing. Reference sample D02 contains a Si/SiO2/HfO2 stack (no annealing), reference sample D03 a Si/SiO2/HfO2/TiN stack (no annealing) and samples D04 and D05 the full Si/SiO2/HfO2/TiN/W stack (D04 pre annealing, D05 post annealing).

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Investigation of a Hypothetical Core Disruptive Accident in Multipurpose hYbrid Research Reactor for High-tech Applications (MYRRHA)

Đ. Petrović, M. Zanetti and G. Scheveneels
Belgian Nuclear Research Centre (SCK CEN), Mol

Dorde.petrovic@sckcen.be

Abstract

Introduction
MYRRHA (Multipurpose hYbrid Research Reactor for High-tech Applications) is a fast neutron spectrum facility cooled by Lead-Bismuth Eutectic (LBE), currently under development at Belgian Nuclear Research Centre (SCK CEN). The main purpose of MYRRHA is to demonstrate the feasibility of an Accelerator Driven System based on a Lead-cooled Fast Reactor. As an ultimate safety barrier in the case of a severe accident, MYRRHA intends to rely on in-vessel retention of the nuclear fuel material. In order to determine the viability of the in-vessel retention strategy, an enveloping case is postulated: the Hypothetical Core Disruptive Accident (HCDA). In the course of the HCDA, core degradation and subsequent fuel relocation are assumed to happen in a way that will lead to a compaction of fissile material with a maximum increase of core reactivity. This further results in a power excursion that leads to coolant boiling and consequent overpressure in the reactor vessel.

Phases of the Hypothetical Core Disruptive Accident
Three phases are considered to describe the HCDA: a core compaction phase leading to prompt supercriticality, a power-buildup phase until delayed supercriticality and a fuel-dispersion phase. The focus of this contribution is on the power-buildup phase. Within this phase, mechanism of reactivity reversal and sequence of events that lead to the disassembly are determined. The reactivity evolution in this phase is driven by a reactivity insertion due to the compaction and countered by the negative reactivity feedbacks due to Doppler effect and thermal expansion of core materials. The power-buildup phase is effectively terminated by fuel expansion due to fuel melting.

Obtained Results and Conclusions
The reference for the phenomena related to the HCDA in MYRRHA was established by employing computer code SIMMER-III. Since the power profile does not change significantly up until the point of LBE boiling, a point kinetics approach can be used to reproduce the reactivity evolution in the power-buildup phase. A simplified approach to analysis of HCDA, based on a coupled neutronic/thermodynamic solver, has been developed at SCK CEN in order to investigate the evolution of reactor core parameters during the power-buildup phase. The core reactivity evolution indicates that the reactivity reversal is caused by the combination of Doppler effect and thermal expansion of the core materials. For large power excursions, further expansion is provided by the fuel melting which rapidly drives the core reactivity to delay supercritical level. Due to thermal inertia, LBE boiling begins during the delay supercritical phase and will result in fuel dispersion, thereby stopping the core compaction. Sensitivity studies indicate that the reactivity reversal mechanism and the sequence of events considered within the power-buildup phase do not depend on the magnitude of the reactivity insertion rate.

Graphene on Si(111) 7x7

Trung T. Pham, and Robert Sporken
University of Namur, Namur

trung.phamthanh@unamur.be

Abstract

Graphene has been proposed as a promising alternative to silicon-based electronics due to its outstanding electrical, optical, thermal, and mechanical properties [1-4]. It opens new possibilities not only for fundamental physics research but also for industrial applications. Since silicon is still the most important single-crystal substrate used for semiconductor devices and integrated circuits, integration of graphene into the current Si technology is highly desirable. A combination between graphene and silicon may overcome the traditional limitations in scaling down of devices that silicon-based technology is facing [5]. Graphene on Si might be one of the most promising candidates as a material for graphene-based technology beyond CMOS. Therefore, it is crucial to find a process to grow/transfer graphene directly on Si. Indeed, there have recently been several attempts to grow graphene on Si wafer [6-9]. However, direct deposition of carbon atoms while maintaining the substrate at a given temperature [7, 8] produces graphene fillms with poor crystalline quality. Further efforts were focused on the direct growth of graphene on Si(111) using a carbon buffer as the solution to reduce the lattice mismatch. Although graphene looks good using this approach, the crystallite size reaches only about 15nm [10-12]. Another one by graphitization of SiC buffer layers preformed on Si wafer [13] requires very high temperature which renders it not directly compatible with standard Si processing technology. It has been proposed to use catalysts on Si wafer [6,14] to reduce the thermal mismatch between graphene and the substrate and to avoid out-diffusion of Si atoms from the substrate during growth. Furthermore, one has tried to exfoliate graphene flakes from HOPG on Si(111) 7×7 substrate using a stamping procedure by means of a wobble stick in a UHV system at room temperature [15]. The advantage of this process is to avoid the physisorbed contaminations and to allow direct covalent bond formation with Si(111) 7 × 7 surface due to its specific reconstruction with unterminated bonds at the adatom positions via the attractive forces such as van der Waals or hydrogen bonds under ambient conditions. However, flake sizes of only a few hundred nanometers are not useful for applications.
Another way to transfer graphene on Si wafer in ambient conditions was reported by Brus et al. [16], where graphene is transferred on top of the

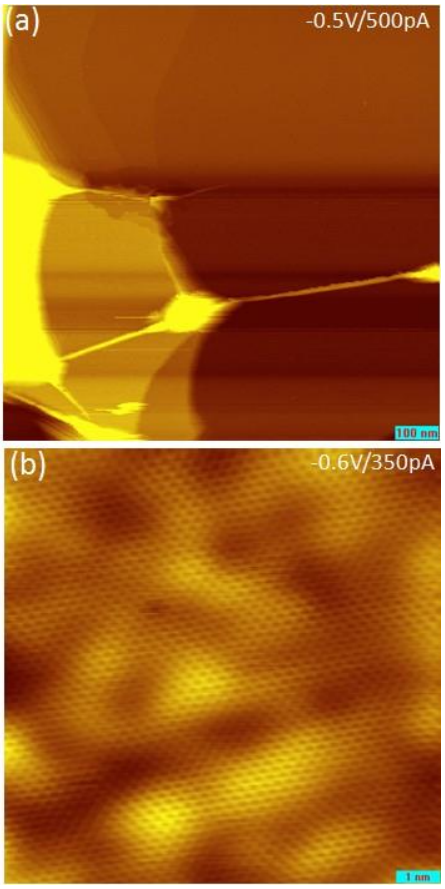

Figure: (a) 1000x1000nm^2 and (b) 10x10nm^2 of graphene on Si(111) 7x7 substrate

CH3 passivated silicon surface from using CVD grown graphene on copper foil. Obviously, this approach required some additional steps of passivation process before the transfer makes it not practical for applications. To overcome the challenges in the transfer of graphene on Si(111), we present here a nice graphene on Si(111) 7x7 substrate (see figure) by means of dry transfer which may be more efficient for device fabrication. Our results are examined by low energy electron diffraction (LEED), Auger electron spectroscopy (AES), Raman spectroscopy (RS), scanning electron microscopy (SEM), and scanning electron microscopy (STM).

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Photonic modeling of two-photon spontaneous emission processes beyond the electric dipole approximation

S. Smeets, G. Rosolen and B. Maes
University of Mons, Mons

Steve.smeets@umons.ac.be

Abstract

We present a framework that can be used to study two-photon spontaneous emission pro- cesses of an emitter near a photonic environment beyond the electric dipole approxima- tion. This is relevant for current nanocavities used for tailoring and enhancing transition rates of spontaneous emission processes. The developed framework is based on the classi- cal computation of Purcell factors and is applied to an emitter close to a silver nanodisk.

Introduction

In this article, we are concerned with the calculation of the two-photon spontaneous emis- sion (TPSE) rates which are 8 to 10 orders of magnitude slower than the competing spontaneous emission of a single photon [1, 2]. In a recent work, it appears that two- dimensional plasmonic nanostructures are ideal to harness TPSE processes from single emitters [3]. Indeed, such systems can confine light in the form of surface plasmons at the atomic scale which leads to a light emission enhancement via the Purcell effect by several orders of magnitude [4]. However, due to this light-confinement, the electric dipole ap- proximation is no longer appropriate [4] because the multipolar processes are enhanced and can eventually dominate [1]. Hence, we present a framework which goes beyond this approximation by considering the contributions of the electric dipole (ED), magnetic dipole (MD), and electric quadrupole (EQ) to the TPSE rate. Then, this one is used to study the enhancement of the TPSE rate of an emitter placed near a silver nanodisk.

Framework

Let's consider a system composed of a quantum emitter placed near a plasmonic nanos- tructure where the interaction Hamiltonian is studied up to the electric quadrupolar order. With a perturbative approach, we know that the probability per unit time that the system carries out a second-order transition by emitting two quanta, driven by virtual intermedi- ate states, is given by Fermi's golden rule. A relation between the TPSE rate of an emitter near an arbitrary object and the corresponding Purcell factors was established for the ED contribution [3, 5]. We have done the same connection for the MD and EQ contributions. For example, the spectral distribution of the EQ contribution to the TPSE rate is given by

$$\gamma_{\mathrm{EQ}}^{(2)}(\omega, \boldsymbol{r}) = \gamma_{\mathrm{EQ},0}^{(2)\cdots}(\omega) \vdots \bar{Q}_{ijkl}(\omega, \omega_t - \omega) \vdots^2 P_{ij}^{\mathrm{EQ}}(\omega, \boldsymbol{r}) P_{kl}^{\mathrm{EQ}}(\omega_t - \omega, \boldsymbol{r}) \quad \rightarrow \quad (1)$$

with $\gamma_{\mathrm{EQ},0}^{(2)\cdots}(\omega)$ the corresponding free-space spectral distribution and $n\omega_t$ the transition energy. For each multipolar contribution, the related equation involves a normalized ten- sor that depends only on the electronic structure of the emitter as well as two Purcell factors which depend solely on the photonic environment. Those factors related to the two emitted quanta of complementary energy can be computed classically.

Application to a silver nanodisk

We consider an emitter placed under a 2D plasmonic silver nanodisk, on its axis of sym- metry. For each multipolar contribution, the normalized tensors are calculated analyti- cally for an s s transition whereas the Purcell factors are computed with the COMSOL Multiphysics® software where classical emitters are modelled by a radiating point ED, MD, and EQ. As the last one is not available, we implemented and tested its weak formu- lation. Fig. 1 shows that the results obtained for the ED contribution correspond to those obtained analytically in [3]. We observe at ω = ωt/2 that the photon-pair emission rate drawn in blue dots is enhanced by, respectively, 5 and 12 orders of magnitude for the ED and EQ two-photon transition with respect to the free-space emission rate.

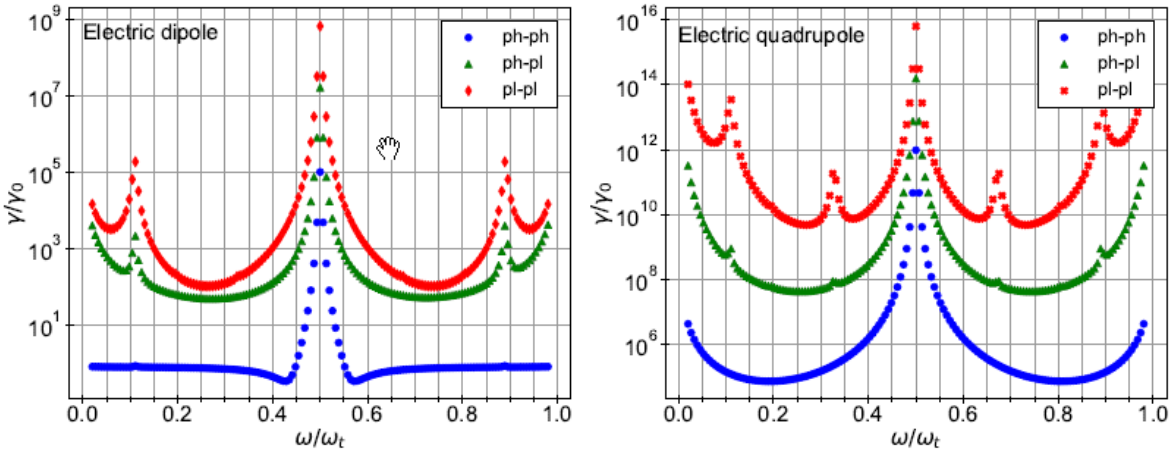

Fig. 1: Photon-photon (ph-ph), photon-plasmon (ph-pl), and plasmon-plasmon (pl-pl) relaxation channels of the ED and the EQ contributions to the spectral TPSE rate between two symmetric states of an emitter. The latter is placed 10 nm above a 25 nm diameter and 4.867 nm thickness silver disk and its transition frequency is n ωt = 2.64 eV.

Conclusion

We developed a framework that can be used to study TPSE processes of an emitter placed near a photonic environment beyond the standard electric dipole approximation. The lat- ter relies on the classical computation of Purcell factors for dipolar electric, dipolar mag- netic and quadrupolar electric point emitters. Finally, we applied the framework to show an enhancement of 5 and 12 orders of magnitude for the electric dipole and quadrupole transitions of an emitter. In the future, the developed framework will allow to study inter- ference effects between the multipolar transition channels of the TPSE processes [4].

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