DCMS MATERIALS 4.0 SUMMERSCHOOL 2017

- The digitally enabled atom to system revolution –

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BOOK OF ABSTRACTS

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(*): also contributed talk

DCMS MATERIALS 4.0 SUMMERSCHOOL 2017

EVENING LECTURE

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Materials Data Space – Roadmap to Industry 4.0-ready Materials

New materials are the key drivers in the development of innovative products in the manufacturing sector. It is estimated that today up to 70 percent of all new products are based on new materials. For industry 4.0, which is the close interlinking of production with the modern information and communication technology, the importance of materials will still rise. Materials should enable future tailor-made products according to individual customer requirements: on demand, adaptive, multifunctional, by design as well as being produced inexpensively, with high quality and with short innovation cycles. To create the digital fundament for materials, the Fraunhofer Group Materials has developed the concept of the Material Data Space®. The Material Data Space® should provide digitally all the relevant information on processes, materials and components in a powerful and perspective company-wide platform, and will allow developers and engineers, to understand the materials used in the respective development steps as variable systems with adjustable properties and use. At the end of the development, a production process could exist where work pieces and products autonomously move through the production lines, i.e., they interact directly with the manufacturing and processing machinery and control their own process. In the lecture, a short introduction to industry 4.0 is given, a proposal for a scientific road map to industry 4.0-ready materials is discussed and the opportunities for material-intensive businesses will be presented.

Biography

Prof. Ralf B. Wehrspohn was appointed jointly by the Martin Luther University Halle-Wittenberg and the Fraunhofer Gesellschaft to work in Halle. As the youngest institute director in the Fraunhofer Gesellschaft, he has headed the Fraunhofer Institute for Microstructure of Materials and Systems IMWS since 2006. He holds the chair of Microstructure-Based Material Design at the Martin Luther University in Halle.

Ralf B. Wehrspohn studied physics at the University of Oldenburg and at the age of 26 received his doctorate from the École Polytechnique in France. At 32 he became a professor of the University of Paderborn. During the period between he worked in industry at Philips Research in London and habilitated (received his post-doctoral qualification) at the Max Planck Institute of Microstructure Physics in Halle.

Ralf B. Wehrspohn's main areas of work are nanostructure materials and components, such as those used in microelectronics, sensors, photonics and in photovoltaics.

KEYNOTE TALKS

SANDRO CARRARA

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Bio/Nano/CMOS interfaces for Ultrasensitive Memristive Biosensors

In this Distinguished Lecture, the very best worldwide ever-reported electrochemical biosensors based on a memristive effect and aptamers or antibodies are presented. These novel sensing devices are developed to propose a completely new approach in the co-design of Bio/Nano/CMOS interfaces for cancer diagnostics. In this research, affinity-based techniques are presented for the detection of the prostate specific antigen (PSA) and the Vascular Endothelial Growth Factor (VEGF). The hysteretic properties of memristive silicon nanowires functionalized with proper biomolecules provide a label-free and ultrasensitive bio-detection technique. In order to develop full systems for diagnostics, the integration with CMOS frontend, in one side of the interface, and microfluidics, in the other side, is required too. Therefore, this lecture also discusses novel circuit approaches for an automated and quick characterization of arrays of memristive biosensors. One memristive parameter, the width of the voltage gap, is directly proportional to the target molecules concentration. Thus, CMOS readouts acquiring such width, meanwhile sorting-out faulty devices, i.e. nonconducting nanowires in the array, are presented together with analog-to-digital conversion for the acquired voltage gap. A prototype of these circuits is shown as an example of design in 0.35µm CMOS technology. The integration of the CMOS readout with the nanoscale sensors and a microfluidic platform is a must for the design of robust biosensing-systems for quick data acquisition in cancer diagnostics. Therefore, the development of an improved chip-platform for cancer diagnostics based on nanofabricated Memristive Biosensors integrated, for the first time, with a microfluidic structure is also presented in this lecture by also addressing critical issues, e.g., the problems related to long connections between the Memristive Biosensors and the CMOS frontend.

Biography

Sandro Carrara is an IEEE Fellow for his outstanding record of accomplishments in the field of design of nanoscale biological CMOS sensors. He is also the recipient of the IEEE Sensors Council Technical Achievement Award in 2016 for his leadership in the emerging area of co-design in Bio/Nano/CMOS interfaces. He is a faculty member (MER) at the EPFL in Lausanne (Switzerland). He is former professor of optical and electrical biosensors at the Department of Electrical Engineering and Biophysics (DIBE) of the University of Genoa (Italy) and former professor of nanobiotechnology at the University of Bologna (Italy). He holds a PhD in Biochemistry & Biophysics from University of Padua (Italy), a Master degree in Physics from University of Genoa (Italy), and a diploma in Electronics from National Institute of Technology in Albenga (Italy). His scientific interests are on electrical phenomena of nano-bio-structured films, and include CMOS design of biochips based on proteins and DNA.

DAVID FIELD

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Heterogeneous dislocation density modeling of interstitial free steel

A polycrystalline interstitial free steel sample was plastically deformed under uniaxial tensile stress at room temperature and a low strain rate. The microstructure of the deformed sample was analyzed using electron backscatter diffraction. In addition, analysis employing a dislocation density based crystal plasticity finite element simulation was conducted using the initial measured microstructure. Both the experiment and the simulation results indicated localized plastic strain and dislocation patterning, which were controlled by the individual crystallite orientations and the grain boundary effects. The results also revealed that the level of concentrated stress at the grain boundaries depends on misorientation at the interface. Grain boundaries and triple junctions had higher hardening effects than the grain interiors as evidenced in both the experiments and model.

Biography

David Field received his BS, MS, and Ph.D. (1991, Yale University) in Mechanical Engineering. From 1990 to 1994 he was employed at Alcoa Technical Center as a Sr. Engineer and from 1994-2000 at TexSEM Laboratories where he was Director of Technology. He joined the School of Mechanical and Materials Engineering at Washington State University in August, 2000.

His research interests include physical and mechanical metallurgy, electron backscatter diffraction (EBSD), deformation and recrystallization of metals, severe plastic deformation, welding and joining, anisotropy of materials, thin film and integrated circuit interconnect reliability, and advanced experimental and characterization techniques. In general, he investigates how to make metals stronger, more ductile, or more corrosion resistant, depending upon the application.

THOMAS HEINE

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Rational Computational Materials Design using Quantum Confinement or Beyond Structural Materials Engineering

Quantum confinement is one of the design principles in nanotechnology. Well-known examples are quantum dots, which are nanocrystals whose electronic band gaps depend crucially on their spatial extension. Thus, it is possible to create light emitting devices with the colour defined by the diameter of the quantum dot. Latest applications include large-scale displays and lasers. In my presentation, I will show that quantum confinement is not restricted to quantum dots and optoelectronic applications. I will show how quantum confinement can be exploited as strategy for the rational design of functional nanomaterials. The first examples are taken from the field of layered materials, where quantum confinement can be used to tailor the band gap, but also the character of the band gap. For example, transition metal dichalcogenides MX2 (M=Mo, W, X=S, Se) are indirect band gap semiconductors as bulk and multilayer phases, but direct band gap semiconductors with appreciable photoluminescence signal as single-layer material. These ultrathin materials are also called two-dimensional crystals. The exploitation of quantum confinement gets even more interesting if the symmetry of the material is changed by changing the layer number. For example, by the absence (monolayer) or presence (bilayer) of inversion symmetry in two-dimensional crystals strong spin polarization effects are observed. The strongest quantum confinement effect so far, we have predicted for PdS2, a two-dimensional crystal that is semiconducting as monolayer, but metallic as bilayer. Similarly, GeP3 is a semiconductor in mono- and bilayer form, but metallic for trilayers and thicker stacks. Another way of exploiting quantum confinement is the application of external fields, most notably electric fields, which are conveniently applied using a gate voltage, and strain fields. I will present various examples where the electronic band gap and/or the density of states are strongly affected by an external gate voltage and by strain fields. For the latter, I will also show some topological phase transitions. In the final part of my presentation I will show how quantum confinement can be exploited to separate isotopes of light-weight elements, e.g. hydrogen or helium. I will present two independent mechanisms that have been realized in metal-organic frameworks (MOFs): MOFs with well-defined apartures that are about the same size as the effective diameter as the dihydrogen isotopologue show a so-called kinetic quantum sieving effect, where the diffusion of heavier isotopologues is favoured. On the contrary, chemical affinity sieving is observed for materials with strong adsorption sites, such as undercoordinated metal ions. Here, the isotopologues have different zero-point energy contributions to the adsorption energy. Using this effect, separation coefficients of 10 and higher can be achieved even at temperatures above 100 K.

Biography

Thomas Heine (born 1970 in Germany) graduated in 1995 in Theoretical Physic s (TU Clausthal, Germany). He obtained his Ph.D. in Theoretical Physics at TU Dresden, Germany, in 1999, working with Gotthard Seifert on the calculation of NMR patterns of fullerenes. Several pre- and postdoctoral stages introduced him into the field of physical and theoretical chemistry. In 2006, he obtained the Venia Legendi in Physical Chemistry from TU Dresden. He was appointed as Associate Professor of Theoretical Physics at Jacobs University Bremen, Germany, in 2008 and was promoted there as Full Professor in 2011. He currently works on the development of density functional theory related methods, metal organic frameworks, spectroscopy simulations and on the electronic properties of low-dimensional inorganic nanostructures.

RICHARD STANLEY WILLIAMS

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The Art and Science of Constructing a Physics-Based Memristor Model

Since the publication of "The Missing Memristor Found" in 2008, there have been many thousands of papers published on the topic of memristors. However, very few of those have featured quantitative compact models of the circuit elements described. This is not a reflection of the maturity of the field but rather the difficulty of constructing an accurate and predictive compact mathematical model for an electronic circuit element that displays memristor behavior. This Lecture will provide a snapshot of the current state of memristor modeling. Such models are essential for designing and simulating complex integrated circuits that contain memristors, and the types of applications being considered are increasing significantly. Although the fundamental equations that specify the device physics may be known, they usually comprise a set of coupled nonlinear integro-differential equations that are extremely challenging to solve in three dimensions, and standard multi-physics solvers may not have all the components needed for an accurate model. A numerical solution of the physics equations can require supercomputers and long execution times, which makes this approach useless for interactive simulation of large circuits that contain many such elements. Thus, the equations must be simplified dramatically, and it is not always clear which terms are the most important for the behavior of the device. On the other hand, a purely black box approach of fitting a set of experimental measurements to a convenient functional form runs the risk of poorly representing the behavior of the device in operating regimes outside the range in which the data were collected. Thus, a hybrid approach is often necessary, in which the mathematical formalism for a memristor provides the framework for the model and knowledge of the device physics defines the state variable(s), operating limits and asymptotic behavior necessary to make the model useful. After describing the challenge, the art and science of constructing a memristor model are illustrated by three examples: a description of a locally active and volatile device based on a thin film of niobium dioxide that undergoes both a thermal instability and an insulator to metal transition because of Joule heating, the original description of a nonvolatile memory device based on titanium dioxide in which the effective width of an electron tunnel barrier is determined by oxygen vacancy drift caused by an applied electric field, and the analysis of a ferromagnetic inductor as a mem-differential element.

Biography

Dr. Williams earned a bachelor's degree in chemical physics in 1974 from Rice University and a Ph.D. in physical chemistry from the University of California, Berkeley in 1978. After graduating, he worked at Bell Labs before joining the faculty at UCLA, where he served as a professor from 1980 to 1995. He then joined HP Labs as director of its Information and Quantum Systems Lab.

INVITED SPEAKERS

DANIEL BALZANI

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Coupled two-scale modeling and simulation of complex materials – Application to multiphase steels

Advanced High Strength Steels (AHSS) are increasingly used in engineering due to their excellent strength and formability enabling e.g. a higher crash-safety in automotive applications. This wide class of steel is characterized at the microscale by a heterogeneous arrangement of different phases, e.g. ferritic/bainitic matrices with martensitic/austenitic inclusions in DP and low-alloyed TRIP steels. These micro-heterogeneities lead to a complex macroscopic material behavior whose phenomenological modeling is difficult. Thus, direct micro-macro calculations often referred to as FE^2 could be applied to not only reliably obtain the macroscopic material response but also to include microscopic physical phenomena into the simulation. These include on the one hand eigenstresses and microscopically graded properties within the individual phases, which could be induced by the production process. On the other hand there may be phase transformations induced by plastic strains in e.g. low-alloyed TRIP steels and microscopic stress concentrations where macroscopic failure may be initialized. Different aspects of AHSS simulations based on this two-scale will be discussed.

Biography

The scientific career of Daniel Balzani, born in 1976, started with finishing his studies on Civil Engineering at the University of Duisburg-Essen in 2003. He accepted the invitation to do his doctoral degree within a DFG research training group at Darmstadt University of Technology which he finished in 2006. Afterwards he returned to Duisburg-Essen to work on his habilitation thesis. In 2009, he was for one year Substitute Professor for Mechanics at the Institute of Mechanics and Numerical Mechanics at the Leibniz University Hannover. In 2010, he worked for 7 months on the basis of a DFG research fellowship at the California Institute of Technology in Pasadena, USA. After that, he finished his habilitation in 2012 and became Professor for Mechanics at TU Dresden in May 2014.

CARLO VITTORIO CANNISTRACI

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Brain active-matter bioinspired algorithms for prediction of self-organization and evolution in complex networks

The brain tissue, as active-matter, is not only inspiration for deep-learning artificial intelligence, but can suggest also other algorithms and paradigms of learning, which are related with its network topology and structural organization. I will discuss the Local-Community-Paradigm (LCP), which is a recent theory we advanced, whose application on real data demonstrates that some basic rules of organization of brain network wiring resemble generalized principles of organization of complex systems to the extent that can be used to predict connectivity in social, economic and biological networks.

The ability to predict new interactions emerges from the structural organization of the complex network that is organized in many local communities inside which the likelihood that a new (or undiscovered) interaction emerges is higher than in the rest of the network. On the basis of this observation, a few years ago we developed the Local-Community-Paradigm (LCP) theory: it suggests that many real complex networks share with the brain a structural organization made by many local communities that favour local signalling activity and then development of new connections within the local communities. This idea was inspired by the famous assumption behind Hebbian learning, a hypothesis advanced by the psychologist Donald Olding Hebb during the late 40s: neurons that fire together wire together, giving rise to new local network connectivity able to implement a process of learning that we called epitopological learning. We proposed also that the identification of this form of learning in neuronal networks was only a special case. Hence, the epitopological learning and the associated local-community-paradigm (LCP) were respectively proposed as local rules of learning and organization, which were proven to be valid in general for modelling link-growth and for topological link prediction in any complex network with LCP architecture.

To conclude, this talk promotes the power of bio-inspired computing, demonstrating that simple unsupervised rules inspired by principles of topological self-organization and adaptiveness arising during learning in living intelligent systems (like the brain) can efficiently equal perform complicated algorithms based on advanced, supervised and knowledge-based engineering.

Biography

In 2005, Carlo Vittorio Cannistraci graduated from the Polytechnic of Milano with a Master degree in Biomedical Engineering. Then he received a six-month research grant from ISIB-CNR, after which he joined the Proteome Biochemistry Laboratory at the San Raffaele Scientific Institute. Since January 2007, he was Ph.D. student of the Scuola Interpolitecnica di Dottorato. In February 2010, he obtained his PhD in Bioengineering under the supervision of F. M. Montevecchi and M. Alessio. From 08/2010 to 01/2014 he was Post-Doc and later Research Scientist in the Integrative Systems Biology Lab. Currently, he is head of the Biomedical Cybernetics Group, Technische Universität Dresden. .

ALESSIO GAGLIARDI

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Simulation of mesoscopic solar cells: challenges and solutions, towards a multiscale approach

A common feature of many novel photovoltaic technologies is that devices present a complex internal structure and an extended interface between different materials. Organic bulk heterojunction [1], dye sensitized [2] and mesoscopic perovskite [3] solar cells all share this feature. The purpose of having a large interface is different in the different devices. In organic solar cells is needed to allow an efficient exciton splitting [1], in dye sensitized to have enough molecular dye and a consequent good light absorption [2] while in perovskite solar cells the advantage of including a mesoporous electron transport layer is still under debate [3]. Whatever is the reason this feature requires improvements in current numerical simulation approaches as the presence of the complex internal interface has a fundamental impact on device performance.

In this talk the state of the art simulation methods for mesoscopic solar cells including the internal morphology are introduced, namely kinetic Monte Carlo and drift-diffusion specifically for organic and perovskite solar cells. It is shown as in organic solar cells the interface plays in fact the major role in device efficiency and it is provided an explanation why mesoporous layers are needed in perovskite solar cells. The various advantages and drawbacks of the two methods are presented and it will be shown a way to overcome the latter using a multiscale approach between the two. This multiscale methodology opens perspectives to simulate many other devices for energy harvesting and storage.

[1] T. Albes, A. Gagliardi, IEEE Trans. Nanotech., 15, (2016) 281-288.

[2] A. Gagliardi et al., Nanoscale 7, (2015) 1136-1144.

[3] E. H. Anaraki et al., Energy Env. Sci., 9, (2016) 3128-3134.

Biography

The research of Professor Gagliardi focuses on nanostructured devices for energy conversion. A major focus of his research is on simulating novel photovoltaic devices, such as dye sensitized, perovskite and bulk-heterojunction organic solar cells using different simulation methods as drift-diffusion and kinetic Monte Carlo. He has also investigated charge transport in single molecule devices for molecular electronic applications using non-equilibrium Green's functions, with particular interest in dissipation at the nanoscale. He is a developer of the TiberCAD and GDFTB software tools. A fundamental area of investigation of his group is multiscale approaches for charge transport, i.e. the way of coupling in a consistent way different numerical models with different level of accuracy to quantitatively address the behaviour of nanostructured devices. After studying engineering in Italy, at the University of Rome Tor Vergata, Professor Gagliardi received his doctorate in physics from the University of Paderborn in 2007 under the supervision of Professor Thomas Frauenheim. He then worked as a postdoctoral researcher at BCCMS (Bremen Center for Computational Material Science). Subsequently (2008) he moved back to Rome where he worked as a postdoctoral researcher in the group of Professor Aldo Di Carlo. In January 2014, he was appointed tenure track assistant professor for simulation of nanosystems for energy conversion at the Technische Universität in Munich in the Electrical and Computer Engineering Department.

MICHAEL GELINSKY

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3D bioprinting of biodegradable implants and tissue constructs

Additive Manufacturing (AM) technologies for biomedical applications have made significant progress in the last couple of years. Whereas patient-specific implants from non-degradable biomaterials like metals or ceramics, e. g. for the treatment of large skull defects, are already state of the art and commonly applied in the clinics, utilisation of resorbable biomaterials is still a matter of research.

We are using multi-channel 3D plotting, an extrusion-based AM technology not requiring complicated or expensive instrumentation and biomaterials which are pasty at room or physiological temperature. These mild process conditions enables the application of a variety of materials like biopolymers, blends and composites and the integration of delicate substances like drugs, growth factors or even living cells.

Recently, we have demonstrated the successful utilisation of several, mostly alginate-based biopolymer blends, biopolymer/calcium phosphate and bioglass composites for 3D plotting and also fabrication of open porous 3D scaffolds from pasty calcium phosphate bone ce-ments. Complex scaffolds with interesting properties can be produced by combining several biomaterials within one construct – either by alternating deposition of respective strands or by combining two materials in a core/shell fashion, using coaxial double needles for extrusion. By alteration of material and morphology, constructs for different medical applications can be produced including scaffolds for the treatment of bone, cartilage, combined osteochondral or soft tissue defects.

Bioprinting – integration of living cells in an AM process – is a fast developing field of re-search. Ink jet-based technologies allow for exact positioning of small cell numbers or cell aggregates, while extrusion-based techniques (like 3D plotting) make use of cells, suspended in hydrogels which are suitable to build three-dimensional constructs by strand deposition. For manufacturing purposes, a sufficient viscosity of the hydrogel is necessary to create open-porous constructs of relevant dimensions. Whereas functional organs still cannot be produced by bioprinting, small tissue equivalents already can be printed. The lecture will give an over-view about the current state of the art.

Biography

Michael Gelinsky has studied chemistry and obtained his PhD at Freiburg University (Germany). In 1999, he moved to TU Dresden and worked for about 10 years at the department of Materials Science, heading his own group at the newly founded Max Bergmann Center of Biomaterials. In 2010, he was appointed as a professor at the Medical Faculty and is leading the Center for Translational Bone, Joint and Soft Tissue Research His work is focused on biomaterials and scaffold development, tissue engineering and regenerative therapies, mostly for musculoskeletal tissues. His group is also very active in the field of additive manufacturing of implants and biofabrication technologies.

TILMAN HICKEL

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Quantum-mechanically guided materials design

An important aspect of the digital transformation in materials science are recent breakthroughs that allow to determine materials properties solely on the computer, i.e. without depending on experimental data. Since this is only possible by understanding and programming the quantum-mechanical foundation of chemical bonds between atoms, such approaches are called "ab initio". There are meanwhile several success-stories where such approaches are used in connection with high-throughput schemas to screen the chemical composition of alloys and which revealed new materials or allowed to optimize key parameters.

In the present talk I will demonstrate that such a screening alone is often only one part of the success. Of equal importance is the fact that ab initio simulations enable us to reveal the physical mechanisms on the atomic scale underlying the macroscopic materials performance. With a focus on steels, we will discuss thermodynamic concepts that determine the phase stability up to the melting point [1]; the role of stacking fault energies for the deformation behavior [2]; the relevance of anharmonic lattice vibrations for the formability of vacancies [3]; and the key parameters determining the solubility of interstitials [4]. The chosen examples will have in common that an introduction into fundamental simulation methods as well as a combination of physical insights and chemical trend studies will be possible thus outlining attractive future prospects connected with Materials 4.0.

[1] T. Hickel, B. Grabowski, F. Körmann, J. Neugebauer: Advancing density functional theory to finite temperatures: methods and applications in steel design, J. Phys: Cond. Mat. 24, 053202 (2011).
[2] O. Güvenç, F. Roters, T. Hickel, M. Bambach: ICME for Crashworthiness of TWIP Steels: From Ab Initio to the Crash Performance, JOM 67, 120-128 (2015).
[3] A. Glensk, B. Grabowski, T. Hickel, J. Neugebauer: Breakdown of the Arrhenius Law in Describing Vacancy Formation Energies: The Importance of Local Anharmonicity Revealed by Ab initio Thermodynamics, Phys. Rev. X 4, 011018 (2014).
[4] U. Aydin, L. Ismer, T. Hickel, and J. Neugebauer: Solution enthalpy of hydrogen in fourth row elements: Systematic trends derived from first principles, Phys. Rev. B 85, 155144 (2012).

Biography

Tilman Hickel graduated in 2001 in Physics at the Humboldt- University Berlin and obtained his Ph.D. 2005 at the same univeristy. Afterwards, he worked as a researcher in the CM department of MPIE, where he became a group leader of the same department in 2006. Since 2008 he is the group leader of ASG Modelling at ICAMS. His focuses are "Ab initio determination of phase diagrams", "Thermodynamics and kinetics of metallic alloys", "Theory of magnetism, many-body theory" and "Shape memory alloys".

CHRISTOPH LEYENS

Institute of Materials Science, Chair of Materials Engineering, TU Dresden and Fraunhofer Institute for Material and Beam Technology - IWS, Dresden
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Additive Manufacturing of Metals: Materials, Processes and Applications

Additive manufacturing of metals is currently paving its way into industrial application at high pace. While in medical applications there is already a widespread use of AM for customized solutions, the strongest innovation boost in AM is coming from aviation industry, followed by the energy sector, automotive industry, space and toolmaking industry.

Using powder bed-based and nozzle-based (wire and powder) AM processes a large variety of customized solutions is feasible, ranging from micrometer-size parts with filigree features to the meter scale of large-size components. With regards to the processing requirements either high accuracy or high productivity can be achieved, whereas a combination is difficult. Among others, examples of industrialized solutions of micro-AM structures for aeroengine use will be given as well as a demonstrator component for space applications with a total diameter of 3 meters.

The presentation will highlight recent developments in AM related to different processes, metal alloys and part sizes/geometries. Unlike any other manufacturing technology, AM of high quality parts requires an in-depth understanding of the close relationship between the AM process, the material and the resulting component properties. As a matter of fact, customized hardware, online diagnostics and control systems are required for robust processing of AM parts. Moreover, the effects of defects on part quality must be studied in detail.

Biography

Born in 1967, Dr. Christoph Leyens studied physical metallurgy and materials technology at RWTH Aachen, Germany, where he earned his diploma in 1993 and his Ph.D. in 1997. He is currently a full professor for materials science and engineering at the Technische Universität Dresden, Germany, and director of the Fraunhofer Institute for Material and Beam Technology, Dresden.

Dr. Leyens has covered a wide range of research topics with a focus on high temperature and lightweight materials, surface technology and additive manufacturing. He has published more than 200 papers, seven books and holds eleven patents.

ALFRED LUDWIG

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Development of new materials using high-throughput experimentation and simulation

The design of new materials is a key challenge in materials science: e.g. new materials for the sustainable production/storage/conversion of energy carriers are necessary to improve existing and to enable future energy systems. Design and of materials includes strategies for efficient discovery and optimization of new materials. A combination of computational and experimental material science, both applying high-throughput methods, is promising. By implementing and optimizing the combinatorial materials science approach in our group during the last ten years, we are trying to contribute to this development. It comprises the fabrication and processing of thin film materials libraries by combinatorial sputter deposition processes (40 elements available) and optional post-deposition treatments (e.g. thermal oxidation, annealing, dealloying), followed by the high-throughput characterization of the different thin film samples contained in these libraries, and in making the next step by the up-scaling of findings from materials libraries to uniform, single-composition samples or to larger, bulk material dimensions. The importance of defining adequate screening parameters and the according design of different materials libraries suitable for one or more screening parameters will be addressed. Our high-throughput material characterization methods are automated, fast, and mostly non-destructive: examples are EDX and RBS for composition, XRD for crystal structure, temperature-dependent resistance for phase transformation, high-throughput test stands for optical properties (color, transmission) and mechanical properties (stress, hardness, elastic modulus), and scanning droplet cells for photoelectrochemical properties screening. The obtained results for ternary and quaternary systems are visualized in the form of composition-processing-structure-function diagrams, interlinking compositional data with structural and functional properties. The talk will cover and discuss examples of the combinatorial development of intermetallic materials for shape memory alloys, superalloys and thermoelectric applications as well as the development of metal oxide thin film materials libraries for solar water splitting. Examples of cooperation with (high-throughput) computational materials science groups will be given. Finally, the importance of developing new materials – not just for themselves but to be part of a system – will be highlighted.

Biography

Prof. Dr.-Ing. Alfred Ludwig received his "Dr.-Ing." from the University of Karlsruhe in 1999. Then he joined the "Center for Advanced European Studies and Research" research group "Smart Materials". From 12/2002 to 09/2007 he was assistant professor for "MEMS materials" at the Ruhr-University Bochum (RUB), and simultaneously head of the caesar research group "Combinatorial Materials Science". From 10/2007 to 10/2012 he was awarded a German Science Foundation (DFG) Heisenberg-Professorship for "MEMS Materials" at RUB. Since the end of 2012 he continues as a full professor at RUB. From 2011 to 2016 he was the coordinator of the "Materials Research Department" at RUB. He initiated and organized the new research building ZGH "Center for interface-dominated high performance materials" in which he serves now as managing director. His research interests include combinatorial and high-throughput methods in materials science, MEMS tools for materials science, nanoscale thin films and multilayers, multifunctional materials as well as new materials for energy applications.

VIKTOR MECHTCHERINE

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3D printing of houses

The talk will provide some insights into the world of modern and future construction materials referring mainly to the key research activities at the Institute of Construction Materials at the TU Dresden. The following topics will be briefly addressed: digital construction with concrete using CONPrint3D technology, virtual concrete lab, carbon concrete composites, textile reinforced concrete, strain-hardening cement-based composites and use of superabsorbent polymers in concrete construction. For every subject, its significance for the practice of construction will be presented and main challenges as well as the scientific approaches to solve them will be outlined.

Biography

Viktor Mechtcherine is Professor of Construction Materials and Director of the Institute of Construction Materials at the Technical University Dresden, Germany. Before that he was Professor at the TU Kaiserslautern (2003-2006) and Chief Research Engineer with the Institute of Reinforced Concrete Structures and Building materials at the Karlsruhe Institute of Technology – KIT (1998-2003). His current research interests include fibre-reinforced cement-based materials, rheology, concrete technology, additive construction, fracture mechanics, durability and new additives and admixtures. He is chair of RILEM TC 260-RSC "Recommendation for Use of Superabsorbent Polymers in Concrete Construction" and member of RILEM Bureau, RILEM Technical Activities Committee, Steering Committee of the fib Commission "Concrete", Editorial Board of the Journal "Cement and Concrete Composites", Editorial Advisory Committee of the Journal "Materials and Structures" and Expert Board "Construction products made of fibre-reinforced cementitious materials" of the German Institute of Structural Engineering (DIBt). Prof. Mechtcherine is Member of Science Academy of Saxony and Russian Academy of Engineering. He is also coordinator of the German Research Society Priority Program DFG SPP 2005 "Opus Fluidum Futurum – Rheology of reactive, multiscale, multiphase construction materials" and speaker of German Research Society Research Training Group DFG GRK 2250 "Mineral-bonded composites for enhanced structural impact safety".

WOLFGANG E. NAGEL

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Biography

Prof. Dr. Wolfgang E. Nagel holds the Chair for Computer Architecture at Dresden University of Technology (TUD). He has studied computer science at RWTH Aachen from 1979 to 1985. Since 1985, he has worked in the area of parallel computing at the Central Institute for Applied Mathematics, Research Center Jülich, and at the Center for Advanced Computing Research (CACR), Caltech. In 1997, he became the founding director of the Center for HPC (ZHR) at Dresden University of Technology (now called ZIH). From 2006 to 2009, he acted as the dean of the Computer Science department at TUD. He is a member of the DFG commission for IT-Infrastructure (KfR), chairman of the Gauß-Allianz, and a member of the International Exascale Software Project (IESP). His research profile covers modern programming concepts and software tools to support complex compute and data intensive applications, analysis of innovative computer architectures, and the development of efficient algorithms and methods.

MARTIN PFEIFFER

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Designing Materials for Organic Photovoltaics

Nanocrystalline layers of vacuum deposited oligomers are known to enable high carrier mobilities parallel to the substrate in field effect transistors. On the other hand, amorphous layers of small molecules with moderate mobilities are widely used for OLED applications. To exploit the attractive features of oligomers for OPV, we obviously need materials with high thermal stability to enable fast thermal deposition and high photo- and electrochemical stability. Moreover, we need to control and manipulate their absorption spectrum, their energy levels and most importantly their preferential orientation and the nanoscale crystallinity and phase separation in blend layers with fullerene C_{60}. The key to get there, is the use of planar A-D-A type oligomers with extended donor block growing preferentially with their long axis parallel to the substrate. The talk will discuss the latest state of the art for a set of absorbers covering the blue/green, red and NIR spectral range, respectively. Recently, pi-stacking perpendicular to the substrate has been achieved leading to further increased fill factors beyond 70%. Furthermore, the current status of multiple junction efficiencies (up to 13.2%), long term durability of flexible samples (up to 7000h in damp heat 85°C/85% r.h.) and of vacuum R2R production is reviewed.

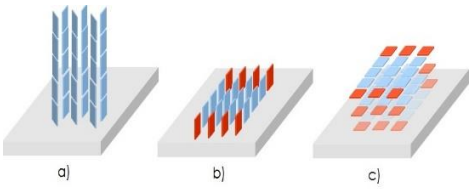

Fig. 1 (a) Typical growth mode of donor oligomers for field effect transistors
(b) of A-D-A-type oligomers for OPV
(c) vertical pi-stacking recently achieved for A-D-A-type oligomers

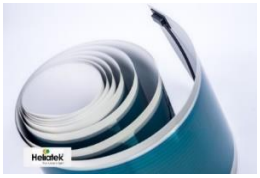

Fig. 2 Flexible solar film produced by vacuum roll-to-roll deposition of oligomer based p-i-n-type tandem junctions. Series interconnection of the cells is done by laser structuring in vacuum within the roll-to-roll process.

Biography

Martin Pfeiffer graduated as a Physicist and is an internationally recognized expert in organic semiconductor technology in the fields of OPVs and OLEDs. Furthermore, he is Co-founder of Heliatek GmbH and Novaled AG, the world leading company in OLED technology.

PEDRO DOLABELLA PORTELLA

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Role of materials data

In a general sense, data are the output of experimental research work. In this workshop we will present some basic ideas concerning the reliability of experimental data; this is a central issue both for individuals or labs producing results as well as for scientists working on theoretical models and engineers designing a machine. Digitalization accelerates enormously the data exchange between these communities; however, the required level of confidence on experimental results increases in the same way. We invite all the participants to reflect upon the value of materials data for their own work.

Failure analysis and prevention – a systematic approach

The advent of the Industrial Revolution was accompanied by several accidents of dramatic dimensions. The analysis of these events was the fundament for the continuous improvement in the reliability of technical systems. In the year 1871 the Prussian state created a technical institution dedicated for this task – the origin of BAM. Failure analysis and prevention is until today a central objective of our institute; due to its complex nature an interdisciplinary task. In our talk we will present an overview of the activities of BAM in the area of failure analysis and prevention; especial attention will be given to the VDI Guide 3822.

Biography

Pedro Dolabella Portella received his Bachelor in Metallurgical Engineering at IME, the School of Engineering of the Brazilian Army in Rio de Janeiro. After nearly two more years at the foot of the Sugar Loaf he received his Master in Materials Engineering at the same institute. In 1984, he received his Dr.-Ing. degree in Erlangen, Germany, with a thesis on high-temperature creep of a Fe-Ni-Cr alloy. After a short stay at the Catholic University in Rio de Janeiro, PUC-RJ, he joined the Federal Institute for Materials Research and Testing (BAM) in Berlin, Germany, in 1987. Since 2000 he is the head of the Department "Materials Engineering". According to the tradition of this institute, one of his concentration areas is failure analysis and prevention. In the period 2010-2011 he was the President of FEMS, the Federation of European Materials Societies. He is an Honorary Member of FEMS, of SPM, the Portuguese Society of Materials, and of SF2M, the French Society of Metals and Materials. In 2010, he received the August Wöhler Medal of DVM, the German Association for Materials Research and Testing, and the Robert Mitsche Award of ASMET, the Austrian Society for Metallurgy and Materials.

FRANK STRIGGOW

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Thinking about your own start-up enterprise - potential support by the Life Science Inkubator

Setting-up and leading your own business to commercial success is a rather extreme challenge. Although this pathway may lead to a high degree of freedom and financial independence, it also poses significant risks. In this talk, conditions and long-term demands of successful entrepreneurship are highlighted. Furthermore, different options for young entrepreneurs to get substantial advice, to raise early-stage financing and to limit financial risks, including some do's and dont's, will be discussed. Finally, demand-tailored support offered by the Life Science Inkubator to potential entrepreneurs and the perspectives resulting from it are presented.

Biography

Dr. Frank Striggow is the Chief Operating Officer of Life Science Inkubator GmbH. He Co-Founded KeyNeurotek Pharmaceuticals AG (Alternate name KeyNeurotek AG) and served as its Chief Executive Officer and President. He is the Site Manager at LSI Sachsen GmbH & Co. KG. Prior to founding KeyNeurotek, Dr. Striggow served as Postdoctoral fellow and group leader at the Institute of Neurobiochemistry, Otto-von-Guericke University Magdeburg and the Julius-Bernstein-Institute of Physiology, Martin-Luther-University Halle/Wittenberg from 1996 to 2001. He also was fellow of the American Heart Association and the German Academic Exchange Service (DAAD), working at the University of Connecticut Health Center, Farmington/USA, and Marine Biological Laboratory, Woods Hole, Massachusetts/USA. Dr. Striggow is author of several publications in international high impact journals, among them Proceedings of the National Academy of Science (USA), FASEB Journal, Current Opinion in Cell Biology, Annals of Neurology and the Journal of General Physiology. Dr. Striggow holds a PhD in biochemistry.

RONALD TETZLAFF

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An Introduction to the Theory of Memristor Cellular Nanoscale Networks

Cellular Nanoscale Networks (CNN) have been introduced by Chua and Yang in 1988 and are characterized by local couplings of nonlinear dynamical systems of comparably low complexity. Since CNN are known as a paradigm for complexity, these networks have been considered in several interdisciplinary investigations ranging from problems in biology and chemistry to the development of high-speed sensor-processor computing arrays with stored programmability. These structures are often implemented on a single chip with optical sensors in CMOS technology and are programmed by CNN templates as instructions in image processing applications e.g. in the real-time control of laser welding processes An introduction to the theory and applications of CNN will be given in this lecture. Especially, memristor CNN will be proposed as new memcomputing structures for future IoT applications. First results will be presented and discussed in detail.

Biography

Ronald Tetzlaff is a Full Professor of Fundamentals of Electrical Engineering at the Technische Universität Dresden, Germany. His scientific interests include problems in the theory of signals and systems, stochastic processes, physical fluctuation phenomena, system modelling, system identification, Volterra systems, Cellular Nonlinear Networks, and Memristive Systems. From 1999 to 2003 Ronald Tetzlaff was Associate Editor of the IEEE, Transactions on Circuits and Systems: part I. He was "Distinguished Lecturer" of the IEEE CAS Society (2001-2002). He is a member of the scientific committee of different international conferences. He was the chair of the 7th IEEE International Workshop on Cellular Neural Networks and their Applications (CNNA 2002) and of the 18th IEEE Workshop on Nonlinear Dynamics of Electronic Systems (NDES 2010). From 2005 to 2007 he was the chair of the IEEE Technical Committee Cellular Neural Networks & Array Computing. He is a member of the Informationstechnische Gesellschaft (ITG) and the German Society of Electrical Engineers and of the German URSI Committee.

POSTERS

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3D Hyperbranched ZnO Nanoarray for Energy and Sensors Applications

Different types of zinc oxide nanostructures (i.e., nanorods and nanofibers) were synthetized, to achieve devices [1], able to work especially as UV sensors [2-6], but potentially also as gas sensors [7-9], or biosensors [10]. Their detection ability was confirmed through multiple analysis, which gave encouraging results for the perspective of progressing these experimentations. Especially, to continue this research in the next future, a combination of these different architectures will be employed. Specifically, the nanostructure architecture which will result, it will be the outcome of implementing nanorods together with nanofibers, to form hyperbranched zinc oxide nanofibers (Fig. 1). These nanostructures were already separately tested, obtaining a clear UV-response behaviour, as result.

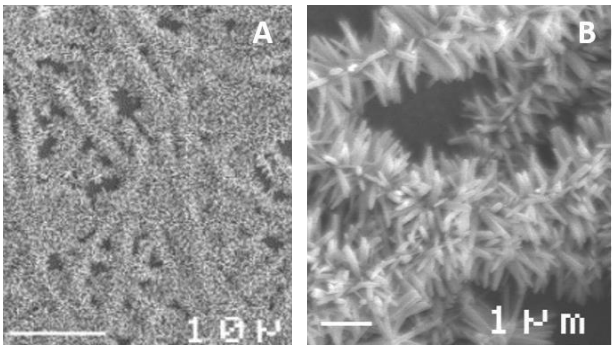

Fig. 1: Hyperbranched ZnO NFs made by growing ZnO NRs on ZnO NFs

This was achieved using a nanofiber-patterned device, not already provided with all wanted nanostructure architecture. But, it has already indeed showed a precise answer, like a relative increase of the electrical resistance of 0.1 when exposed to UV illumination under an applied bias of 1.5 V. If it would be considered that tested device was not arranged with an all-complete set- up, these results are really promising, even if they are surely need to be increased. The obtained zinc oxide nanostructures will be also tested to evaluate their antimicrobial properties, in order to use them in surfaces or coatings, within the wider strategy against nosocomial infections.

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Monte Carlo simulations of 2D molecular self-assembly of Pentacene

Controlling the formation mechanism of organic thin films (OTFs) tailored by weak interactions on van der Waals (vdW) substrates provides an opportunity to obtain highly stable, large-area, and high-quality organic electronic devices [1]. To this end, understanding the self-assembly of organic molecules, like pentacene, from a disordered state into ordered 2D crystals is of great importance. The aims of this study are (1) identify intrinsic driving mechanisms responsible for the molecular ordering and (2) analyze the role of the substrate for the growth process. Our work complements a recent study based on molecular dynamics simulations[2].

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FRANCESCO DECATALDO

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PEDOT:PSS: an organic semiconducting material as cell culture substrate to monitor tissue integrity

Semiconducting polymers are very promising materials for biomedical application, thanks to the ability to conduct both ions and electrons, their biocompatibility and their flexible and soft mechanical properties. In particular, poly(3,4-ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT:PSS) has high conductivity, electrochemical and thermal stability in aqueous environment and low oxidation potential that renders it suitable as interface with biological environment.

In our work, PEDOT:PSS thin films are used as cell-culturing material for different kind of cells (HeLa, NIH-3T3) and represent the channels of Organic Electrochemical Transistors (OECTs). In our devices, the electronic current flowing in the conducting polymer channel is modulated by the ionic current crossing the interface with an electrolyte solution (cell culture medium). The presence of a cell monolayer at this interface slow down the ions flowing in the conducting polymer, thus providing an electronic readout of the layer integrity.

Electrical monitoring is based on two parameters: the current modulation and the response time of the OECT to a potential step applied to the gate. We find that these parameters are quantitatively related to cell layer integrity and confluence.

We demonstrate that PEDOT:PSS allows cell growth and adhesion on its surface, without the addition of process able materials that promote cell attachment, and that our devices provide a fast and dynamic method to monitor cell viability and reactions to toxic agents, paving the way for high throughput and low-cost screening of drug discovery or toxicology.

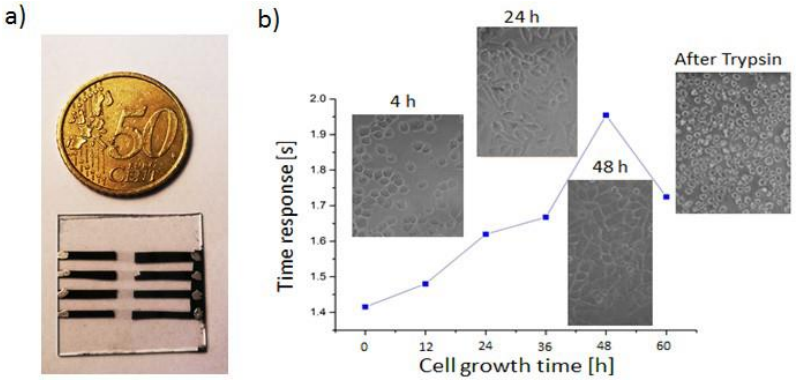

Fig.: *a) Photo of the channels of the device, with the thin Pedot:Pss film connecting gold stripes, used as source and drain; b) Response time of organic electrochemical transistor at different cell coverages (HeLA) on the PEDOT:PSS channel and after the use of Trypsin-EDTA (an enzyme that detaches cells from the substrate).*

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Surface functionalization by soft landing for sensor and antenna applications

This thesis deals with the development of a new kind of physicochemical sensors using high frequency characteristics, and based on an original deposition technique: the mass spectrometer. This chemical analyze machine, used to perform the analyses of the materials by ionization, has been deflected from its original application and applied for the deposition of reactive thin films. Therefore, the mass spectrometer will permit the fabrication of sensitive layers. This first step will be followed by the design, fabrication and characterization of the antenna systems integrating the sensors.

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Manufacturing of porous models for investment casting for heat storage application

Phase Change Materials (PCMs) can be used in heat storage supporting many industrial processes e.g. recovering waste heat sources or absorbing the excess of energy in the form of latent heat of fusion. Although their thermal conductivities are relatively low (e.g. 0.2 W/mK for paraffin, 0.4 W/mK for KNO3, 0.5-0.6 W/mK for NaNO3) what prolongs the charging/discharging cycle of the heat accumulators. In order to improve heat transfer within PCM, differently shaped metal structures were developed and can be immersed in the PCM material. Cellular metals can be applied for heat exchangers, radiant burners in combustion engines, battery electrodes, flame arresters, acoustic dampers. Porous metal structures can be obtained via investment casting technology with the use of polyurethane replica models. This technique is based on manufacturing of metal foams reflecting the shape of polyurethane foams of different levels of porosity (10, 20, 30 ppi – pores per inch). This model can be modified and adjusted in order to improve the heat transfer parameters (heat conductivity, specific heat transfer area). Porous structures were impregnated with paraffin or potassium nitrate KNO_3 and an experimental test stand was built to study the heat transfer characteristics of composite PCMs. Performed multiple heating/cooling cycles confirmed the high transfer of heat and good stability of the system.

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Efficient Simulation of Additive Manufacturing Processes

As Additive Manufacturing (AM) is becoming more cost effective its role as a manufacturing process will increase. To ensure the quality especially of performance-critical components realiable and time efficient simulation is necessary. Current developments in spatial adaptivity shall be applied to the simulation of additive manufacturing to further improve those methods.

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Quantum Phases of Spin ladders with Skewed Rungs

Heisenberg Antiferromagnetic (HAF) spin chains have been studied for a long time[1-3]. Frustrated HAF with next near neighbour antiferromagnetic interactions are also well known [4-9]. Linear chains of spin-1/2 systems are gapless system realized in crystals containing spin 1/2 transition metal ions. Haldane claimed the spin-1 chains to be gapped systems as was soon confirmed numerically as well as experimentally. The quantum phases of nearest and next nearest spin chains were studied extensively and was found to exhibit gapless as well as gapped and spin spiral phases. In recent years studies on spin chains are focused on exotic phases and the possibility of multiferroic materials. In order to explore these possibilities we have incorporated geometrical frustration into spin-1/2 ladders by introducing skewed rungs. Chemically these represent fused conjugated systems. In this study, the quantum phases of 2-leg spin-1/2 ladders with skewed rungs are obtained using exact diagonalization of systems up to 26 spins and density matrix renormalization group (DMRG)calculations to 500 spins. These systems show high spin ground states with the spin increasing within creasing system size. Some of them also exhibit re-entrant singlet phase. I will discuss the magnetic ground state of fused azulene (5/7 membered ring) in particular and fused frustrated ring systems (e.g.3/5 and 3/4 systems) in general.

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Phase Field Model for Interface Failure

A phase field model for interface failure between two materials is proposed where the interface is incorporated by a local reduction of the critical fracture energy. Due to the use of a regularised crack model, interaction between the length scales of the crack and the material interface has to be analysed. A local approach is presented, that compensates the influence on the actual fracture toughness at which the crack propagates along the interface.

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Complex structural characterization of glassy carbons and correlations structure – mechanical properties

Glassy carbons are a class of non-graphitizing, nanoporous carbons widely used in a range of applications due to their unique combination of properties such as high thermal and chemical stability, low density, impermeability to gases, high tribological performance, and biocompatibility. However, the atomic arrangement of glass-like carbon is complex, strongly depends on the carbonization conditions, and causes difficulties in its structural characterization. Particularly, there are no commonly adopted model of the nucleation and growth of curved structures in glassy and other pyrolyzed carbons. The most recent studies have suggested that glassy carbons have a fullerene-related atomic structure [1].

We try to establish structure-properties correlations of a series of glass-like carbons produced by pyrolysis of polyfurfuryl alcohol and go beyond the previous studies. Given the complexity of considered materials and their sensitivity to the synthesis temperature we used characterization based on many experimental techniques (X-ray diffraction, Raman spectroscopy, transmission electron microscopy, electron energy loss spectroscopy, nanoindentaion) as well as theoretical simulations of atomic structure. The combined studies allowed a detailed structural specification of the investigated carbons and offered new models of atomic arrangements that can explain the origin of their properties. We noticed that the presence in glassy carbons of postulated topological defects and curvature has a distinct manifestation in the diffraction data [2]. A gradual reduction of curvature in fullerene-like fragments of the structure and elimination of related defects accompany the increase in heat-treatment temperature. We are able to show how these changes directly affect mechanical properties.

Since the structure is a key parameter determining glassy carbon porosity, chemical, mechanical and electronic properties, the possibility to control the temperature-induced structural transformation is critically important for the fabrication of the glassy carbon products with desired functional features.

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DORON KAM

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Cellulose nanocrystals for 3D printed objects

Direct ink writing (DIW) is an extrusion based 3D printing technique where design model can be assemble into 3D objects. As compared to other 3D printing methods, in DIW the material is liquid to gel and flow throw nozzle. The ability to build a new layer on top of another layer leans on the ability to cross-link the material mainly by physical or chemical approach. Our approach is to use cellulose nanocrystal (CNC) as an ink for DIW, while using it's unique rheological property that allows printing CNCs 3D hydrogel objects.

Cellulose nanocrystals (CNCs) are rod-like, nanometric-sized, crystalline components, made from the hydrolysis of natural cellulose sources. Differences in hydrolysis conditions influence CNC properties, including size, surface charge, phase behavior, and rheology. Understanding of the relationship between preparation conditions and resulting properties is significant for designing CNC applications. For instance, the shear-thinning rheological behavior of CNC suspensions is attractive to the paint industry, since under the application of shear, viscosity drops and the paint is applied smoothly, but once the shear is stopped, paint viscosity increases, preventing dripping. This fundamental rheological behavior is the key parameter for DIW, while applying shear force material is liquid and when material is out of the nozzle viscosity goes up and printed layer can maintain more layers on top.

To preserve printed 3D structure of pure CNC one could let the sample self-assemble or freeze dry the sample into foam. Printing CNC 3D foams has various application from tissue engineering and biomedicine to packaging and beyond. This environmentally biological biodegradable 3D foam, plays as a replacement for nonbiodegradable petroleum derived foams and as a novel approach in 3D printing.

CNC 3D printed hydrogel designed as Werther's Original candy

CNC 3D printed foam designed as Werther's Original candy

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Martensite Gradient in DP980 Dual Phase Steel

Dual phase (DP) steels have provided high strength solutions to the automotive industry, allowing for safer cars while reducing weight and improving fuel economy [1]. In addition, the advantages of grain size gradients in the strength of metals have been shown through improved fatigue characteristics. By creating nano-crystallized surface grains increasing towards the core of the material, the ductility and strength can both be increased [2,3]. The purpose of this project was to generate a martensite gradient in DP steel. Samples that were furnace cooled and ice-water quenched from 790° C and as received showed average Rockwell C hardness values of 35.7 HRC (0.45 std. dev.) and 24 HRC (1.2 std. dev.) respectively. Quenching one end of the sample while allowing the other end to cool in air resulted in an equivalent maximum hardness, with a lightly increases minimum hardness (29.5 HRC). A gradient over a shorter area was formed by heating only one end of the sample and then quenching in ice water. This allowed the transition to be imaged via chemical etching and optical microscopy. Surface deformation using shot peening was not found to have any significant effect on grain size. More severe plastic deformation, such as surface mechanical attrition treatment (SMAT) or high-pressure torsion (HPT) is an area of interest in future work of this project.

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Multiscale computational design of metal-ceramics joining process

In modern times, the integration of new materials into usable products has a special relevance for the technological development and economic competitiveness of industrial societies. High-temperature applications in aeronautics, space, energy and nuclear power require advanced ceramics. In all these applications, the high-temperature environment is present and ceramics are one of the choices since they retain stiffness and strength at high temperatures. Also, they have much better high temperature creep resistance than metals. Structural ceramics are developing rapidly and they are most commonly used as wear parts or parts of energy-production systems. However, near net shape ceramic parts are difficult and expensive, sometimes even impossible, to manufacture. Therefore, joining of components is necessary. Joints are the weak link since the range of operational temperatures of a part is determined by the joint and is significantly lower than the base material (ceramic) could withstand. Therefore, designing joints is essential for high T applications. The desirable joint, in this case, is the seamless homogeneous bond with minimal internal stresses. The current joining process design methods do not solve this issue correctly since they limit the operating temperature or produce significant residual stresses and they are largely based on experience. Finding a method that can predict the behavior of the joints and produce seamless homogeneous bond based on a limited set of experimental input data is highly desirable. It would have a breathtaking impact on the industrial societies.
The main goal of this research is to develop a computational procedure, based on a set of experimental data for predicting the microstructure of ceramic-transitional and metal-ceramic joints. The computational method for mesoscale will be the phase-field method which will consider the internal stresses in the joint and the surrounding material arising from thermal expansion mismatch, compositional strains and the phase transformation strains. Thus, the major modeling challenge is the definition of the optimal phase-field formulation. The complex diffusion and phase transformation processes can be simulated with various levels of complexity. The increased complexity carries the increase in both, the computational cost, and the cost of additional experiments required for additional parameters. So, determining which aspects of the problem are essential and which are marginal is of great value.

In order to calibrate the numerical model, the joining of ZrC*x* parts via a Ti interlayer will be considered. The active diffusion bonding procedure applied to this combination of materials can produce a variety of interface microstructures (including the seamless joint with the total dissolution of the interlayer), depending on carbon concentration, joining temperature, time at the peak temperature, and thickness of the Ti interlayer. In the same step, the range of parameters of the joining process which produces the seamless homogeneous bond will be defined. When numerical accuracy is reached, the other combinations in addition to ZrC*x* will be made using the following candidates: TiC*x*, HfC*x*, TaC*x*, and NbC*x*, with a metallic interlayer. Diffusion kinetics and thermodynamics of the interfacial elements and carbon vacancies will be modeled and compared with the experimental results.

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Prediction and Fabrication of Materials With High Piezoelectric Coefficients and Flexibility

Computational chemistry tools would be used to run simulations for predicting piezoelectric coefficients of novel piezoelectric materials. This would be used to select polymers or polymer composites with the right characteristics for large-scale energy harvesting from vibrations. These characteristics include: high piezoelectric coefficient, flexibility, and high power efficiency. While piezoelectric crystals have higher piezoelectric coefficients, they tend to be brittle. On the other hand, piezoelectric polymers are flexible but tend to have lower piezoelectric coefficients. Internally-charged electret polymers and polymer composites, which are made up of a polymer and a crystal, show the most promise for meeting the criteria of high piezoelectric coefficient and flexibility. Fabrication techniques like e-beam evaporation would be used to produce thin films out of the chosen materials. Finally, the fabricated devices would be tested to validate their molecular structure and measure piezoelectric coefficients.

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Seperation of Oxygen Vacancy Defect Levels in the Ultrathin SiO_2 Interfacial Layer of High-k/Metal Gate CMOS Devices

The reduction of the system size is driving the conventional gate dielectrics to their physical limits. Thereby excessive gate leakage current and reliability issues are of special interest. In this context oxygen vacancy defect levels in ultrathin SiO2 layers in metal-oxide-semiconductor devices were investigated. For Si/SiO2/HfO2 gate stack and a SiO2 bulk reference system first principles calculations were performed. We find that a energetic level splitting and stabilization of certain SiO2 bulk defects is caused by a symmetry break, which results from the small interfacial layer thickness and dissimilar structural and electronic properties of the adjacent layers (namely Si and HfO2) in state-of-the-art gat stack systems. It could be shown that a partial H passivation of the vacancies stabilizes those defects energetically which are related to the leakage current in CMOS devices.

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Molecular dynamics simulations of pressure-induced structural and mechanical property changes in MgSiO3 glass

Molecular dynamics simulations of MgSiO3 glass have been carried out to investigate the pressure-induced structural transformation and mechanical properties. The local atomic structure was analyzed through the pair radial distribution functions, bond angle distributions, coordination number, void statistics and common neighbour analysis. With increasing pressure, O atoms are more ordered than Mg and Si atoms and to form faced centered cubic (fcc) or hexagonal closed packed (hcp) clusters. The change of local atomic structure upon compression has been also presented. The mechanical properties are also discussed in detail.

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Group-V elemental bilayers: A tunable structure model with four-, six-, and eight-atom rings

Two-dimensional (2D) group V elemental materials have attracted widespread attention due to their nonzero band gap while displaying high electron mobility. Using first-principles calculations, we propose a series of new elemental bilayers with group V elements (Bi, Sb, As). Our study reveals the dynamical stability of 4, 6, and 8-atom ring structures, demonstrating their possible coexistence in such bilayer systems. The proposed structures for Sb and As are large-gap semiconductors that are potentially interesting for applications in future nanodevices. The Bi structures have nontrivial topological properties with a direct nontrivial band gap. The nontrivial gap is shown to arise from a band inversion at the Brillouin zone center due to the strong intrinsic spin-orbit coupling (SOC) in Bi atoms. Moreover, we demonstrate the possibility to tune the properties of these materials by enhancing the ratio of 6-atom rings to 4 and 8-atom rings, which results in wider nontrivial band gaps and lower formation energies.

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Dirac fermions and pseudomagnetic fields in two-dimensional electron gaseswith triangular antidot lattices

We investigate theoretically the electronic properties of two-dimensional electron gases (2DEGs) with regular and distorted triangular antidot lattices. We show that the triangular antidot lattices embedded in 2DEGs behave like artificial graphene and host Dirac fermions. By introducing the Wannier representation, we obtain a tight-binding Hamiltonian including the second-nearest-neighbouring hopping, which agrees well with the numerically exact solutions. Based on the tight-binding model, we find that spatially nonuniform distortions of the antidote lattices strongly modify the electronic structures, generate pseudomagnetic fields and the well-defined Landau levels. In contrast to graphene, we can design the nonuniform distortions to generate various configurations of pseudo-magnetic fields. We show that the snake orbital states arise by designing the $\pm\mathbf{B}$ pseudo-magnetic field configuration. We find that the disorders of antidot lattices during fabrication would not affect the basic feature of the Dirac electrons, but they lead to a reduction in conductance in strong disorder cases.

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The development of additive manufacturing technique for nickel-base alloys: a review

Nickel-base alloys are an attractive alloy due to its excellent mechanical properties, a high resistance to creep deformation, corrosion and oxidation. However, it is a hard task to control performance when casting or forging for this material. In recent years, additive manufacturing (AM) process has been implemented to replace the conventional directional solidification process for production of nickel-base alloys. Due to its potential lower cost and flexibility manufacturing process, AM is considered as a substitute technique for the existing. This paper provides a comprehensive review of the previous work related to the AM techniques for Ni-base alloys while highlighting current challenges and methods to solving them. The properties of conventionally manufactured Ni-base alloys are also compared with the AM fabricated alloys. The mechanical properties obtained from tension, hardness and fatigue test are included, along with discussions of the effect of post-treatment process. Recommendations for further work are also provided.

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Innovative TiO2/Poly (vinylidene difluoride) coating of polymeric optical fibers for enhanced photocatalysis

In this work, the photocatalytic efficiency of TiO2 P25 immobilized in a poly (vinylidene difluoride) matrix coated on polymer optical fibers (POF) by dip-coating, under visible light were characterized and evaluated. The coatings were characterized by tape testing and SEM/EDX. The photocatalytic efficiency was assessed by analyzing the degradation of ciprofloxacin and the reusability was tested. The results showed that 17 w/w % of TiO2 P25 achieved a degradation of 95 % after 72 hours under simulated visible light and its reusability was tested for 3 times with a loss of activity lower than 11 %. The efficient removal of ciprofloxacin and the reusability tests demonstrated the suitability on the degradation of pollutants and the stability of the POF coated with TiO2 P25 in water treatment. To the best of our knowledge, PMMA-POF coated by TiO2/PVDF and the reusability of any type of POF for photocatalytic applications has not been reported previously.

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Solvent effects on the electronic transport properties of graphene

Graphene has the potential to induce significant change in the way we construct and use electronic devices. However, on the one hand, the presence of water molecules - even at low concentrations – is unavoidable, and such effects on the electronic transport properties could be significant. On the other hand, many possible applications include biological systems or molecules in solution. In those cases, the device is embedded in an aqueous solutions. The effects of this solutions is not fully known, and from a computational point of view, is quite challenging.

The methodology known as QM/MM is very useful for modeling large systems as realistically as possible. In our case, a periodic simulation box with graphene, water molecules and counter-ions (NaCl) sampled via Molecular Dynamics can be divided into a classical and a quantum part. The solvent can be treated by molecular mechanics methods while the graphene sheet must be treated quantum mechanically (via Density Functional Theory), since we want to investigate the electronic transport throughout the sheet. Finally, the electronic transport properties are obtained via the Non-Equilibrium Green's Functions formalism.

Thus, in this work we will present an extensive investigation of the electronic transport properties of solvated graphene using this technique. We performed simulations of graphene in different solvation conditions by varying the concentration of NaCl. We also tested the rigid rod model for polarization in graphene, as implemented in GRAPPA force field, in order to improve the description of the liquid-graphene interactions. Our results show that the electronic transport properties of solvated graphene are not very sensitive to salt concentration, even in high concentration. The overall trend for the presence of water is to induce a chemical gating effect that shift the local Fermi level of graphene, leading to doping of the sheet.

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Multi-layered composite materials of new generation energy-absorbing electromagnetic waves of civilian and military application

Developed manufacturing technology of multilayer composites of the new generation may be interesting for government (magnetically sealed construction of government buildings such as ministries, embassies), banks, insurance companies, boards of companies working in the field of high-tech, but also the inhabitants. The technology will protect objects from electromagnetic radiation coming from the outside, as well as it limits the range of electromagnetic waves emitted inside the building. The aim of the research is to produce a multi-layer composite materials containing the absorber of electromagnetic radiation. In addition to the properties of electromagnetic waves absorption produced composite is characterized by an increased impact resistance, abrasion resistance and will possess a very good adhesion to the substrate steel and polymer. In addition, it will be resistant to weathering and chemical agents. This goal will be achieved by the development of composite materials suppressing electromagnetic waves consisting of a layer of steel or polymer, an absorber layer, a layer of Kevlar, a layer of elastomer.

The electromagnetic absorbers may be used in:

1. military technology,
2. telecommunications,
3. electronics and consumer electrical appliances,
4. electrical engineering,
5. energetics,
6. ISM equipment (industrial, scientific, medical),
7. measuring laboratories.

New absorbent materials allow a significant improvement in the attenuation of electromagnetic waves and the operation of the equipment and systems. An important feature of the innovation of new generation materials is the fact that by:

- altering in any way the final compositions of materials,
- changing the processing conditions during the preparation of these materials or
- forming of the final materials in the preparation of the final product multilayer systems of different absorbencies hybrid products can be obtained with specific desired both in terms of the magneto-dielectric and physical properties.

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Multiscale modelling of heat conduction in 2D materials and heterostructures

Over the last couple of decades, there have been tremendous efforts for the fabrication of two-dimensional (2D) materials. Graphene, hexagonal boron-nitride (h-BN) and molybdenum disulfide (MoS2) are revolutionary 2D materials with remarkable properties, proposing them as unique candidates for a wide variety of application from post-silicon electronics to aerospace structures. Nowadays, chemical vapour deposition (CVD) technique is the only way for producing large-scale films of mentioned 2D materials. In principal, CVD is also considered as the most promising method to construct lateral and in-plane heterostructures of 2D materials. During the CVD growth, crystal growth initiated from nucleation sites leads to the construction of polycrystalline structures. Consequently, CVD grown 2D films are consisting of different grains that could be distinguished by existing grain boundaries. These grain boundaries throughout the CVD grown films include various types of topological defects. In the CVD grown structures, by decreasing the grain size, more grain boundaries form which accordingly increase the defects concentration throughout the sample. Like all known materials, these defects can affect the material properties. Defects along the grain boundaries cause stress concentration and phonon scattering resulting in lower mechanical and thermal conduction properties. Accordingly, a comprehensive understanding of grain size effect on the properties of CVD grown films is of crucial importance. The objective of this work is therefore to provide general viewpoint concerning the heat transfer along several 2D polycrystalline and heterostructure films. In this investigation, we explore the thermal conductivity by developing combined atomistic-continuum multiscale methods. We particularly study the thermal conductivity of polycrystalline graphene, h-BN and MoS2 membranes. In addition, we explore the thermal conductivity along graphene/h-BN in-plane polycrystalline heterostructures. Next, we study the thermal conductivity of graphene or h-BN laminates. We finally discuss that the proposed multiscale modelling schemes based on the atomistic and continuum modelling can be considered to accurately explore the effective thermal conductivity of various 2D structures with complex atomic structures and grain boundaries.

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Enhanced Mechanical Robustness of Vertical Graphene Sheets by Ion Bombardment and Fluorination

Graphene, a material whose remarkable properties make it supremely desirable for a wide variety of applications can benefit from both physical and chemical modifications. In this work, we report the effects of controlled defect creation facilitated by ion-beam irradiation and the addition of fluorine on the vertical graphene (VG) sheets, introduced by a XeF2 etching system. An increase in the average effective reduced modulus (*Er)* from 4.9MPa for pristine, as-grown sheets, to 10.0Mpa and 18.4MPa after irradiation and fluorination respectively was observed. The combined effects of both bombardment and fluorination was seen to produce a maximum *Er* of 32.4MPa. These dramatic changes can ultimately be explained by the introduction of covalent bonding between the VG sheets through irradiation and increased corrugation due to fluorination. We thus illustrate that both defect creation and chemical functionalization can be applied to manipulate VG sheets' mechanical properties and can work simultaneously to achieve the largest enhancement of the mechanical stiffness. This tailorable feature can be used in applications where particular mechanical properties are desired.

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3D Hybrid Skin Implants

The lack of skin protection in case of injury can cause patients a severe infection, pain and suffering. Furthermore, scarring can cause external deformation and therefore heavy mental suffering. A three-dimensional custom made hydrogel is developed via 3D printing method, resulting in tunable controlled implant geometry and porosity as a treatment for soft tissues injuries and cosmetic cover of skin deficiency.

The hybrid implant will possess high biological compatibility, controllable mechanical and gas barrier properties. The implant is designed and engineered to be temporarily in order to allow patients an immediate solution. The implant assembled from three layers: Adhesive layer, hydrogel matrix and hydrophobic outer layer.

1. Adhesive layer adhere to the skin and can be removed
2. The hydrogel matrix composed from poly (vinyl alcohol) (PVA) and biomaterials such as recombinant human (rhCollagen) protein and cellulose nanocrystals (CNCs)
3. The outer layer composed mainly from biomaterials that can be found in the epidermis such as keratin and melanin.

The research focuses at each layer individually and at the interaction between them.

We are aiming to mimic the skin properties and function along the complex skin texture. To ensure high level of skin implant we are exploring the combination of different biomaterials following advance processing methods such as 3D printing.

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3D printing in pharmaceutical industry and 4D printing as biofabrication next generation

Layer-by-layer fabrication of 3D objects from digital models is called 3D printing. This technology established three decades ago at the confluence of materials science, chemistry, robotics, and optics research to ease the fabrication of UV-cured resin prototypes and rapidly considered as a standard instrument in the aerospace, automotive, and consumer goods production factories. Nowadays, 3D printing has achieved traction in the pharmaceutical industry demonstrated in August 2015 by a 3D-printed FDA approved drug product. This scientific contribution summarizes advancement in 3D printing of drug products and discusses 4D biofabrication as the next generation technology.

The traditional pharmaceutical methods such as granulation or tablet compression, have been used for decades and are well understood, however, antiquated in terms of production flexibility and process effectiveness. As a novel manufacturing method, 3D printing has competitive advantages for made on-demand, personalized and complex products that establish opportunities for enhancing the accessibility, effectiveness, and safety of drugs. However, there are some limitations associated with current 3D printing methods and products in biomedicine applications, originated from the static characteristics and behaviours of current 3D printed structures and products. This scientific contribution illustrates how a control strategy development can be facilitated by process and product realization for the various 3D printing techniques. Also, it demonstrates how dynamic 3D printed products can be created using developed 3D strategies and stimuli responsive materials to overcome the associated limitations with conventional 3D printers. In the other words, the study begins with a review of different 3D printing technologies used in drug production industries, and compare them with traditional pharmaceutical methods, to explain the potential effect of 3D printing on drug delivery systems, complex, personalized/ made on-demand products, and clarify the future of 4D bio-printing as a novel method to mimic the dynamics of a native tissue.

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First Principle Calculations on Thermoelectric Properties of Monolayer Transition Metal Dichalcogenides

Investigations of the thermoelectric effect in monolayer transition metal dichalcogenides (TMDs), which provides conversion of heat into electrical current or vice versa, is a highly active research area in recent years. An efficient thermoelectric material requires a remarkable increasing electrical conductivity and reduced lattice thermal conductivity. However, enchancing the efficiency of thermoelectric material is rather difficult because the electronic thermal conductance (κe), lattice thermal conductance (κph), Seebeck coefficient (S), electrical conductance (Ge) and power factor (P) are mutually coupled coefficients entering the thermoelectric figure of merit ZT. Therefore, researchers tend towards exploring the new members of potential thermoelectric material candidates as well as obtaining maximum ZT value by nanoengineering.

Electronic and phononic properties of MX2 (M = Ti, Zr, Hf, Cr, Mo, W, Mn, Tc, Re; X = O, S, Se, Te) monolayers are investigated for phases with various symmetry groups such as 2H, 1T , 1Td and 1Td´. All electronic calculations are perfomed by using VASP package. Force constants are obtained by using density functional perturbation theory (DFPT) as implemented in the PHONOPY code. Landauer formalism is used for thermoelectric coefficients of dynamically stable TMDs at the ballistic limit. Aforementioned materials are classified according to their thermoelectric efficiency and resulting ZT values get enhanced without any nanostructuring.

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Polymeric Ultra-thin PDMS Membrane (PUMs): synthesis, characterization and integration in Lab-on-a-Chip devices

The aim of my PhD project is to demonstrate a computing paradigm based on charge confinement and electrostatic interaction between neighbouring molecules inspired on *Quantum Cellular Automata* (QCA) model. In the novel architecture, the molecules are self-assembled onto the device surface without nanoscale lithography and clocking of the device that controls information. Propagation is implemented electrostatically through gradients in the thickness of the dielectric layers within the device. Therefore, we will refer to the new model of computing paradigm as *Molecular Functional Cellular Automata* (MFCA). Scientifically, the proposed strategy rests on three, tightly connected pillars:

(i) Tailored design of molecular systems suitable for MFCA applications and their molecular assembly in ordered molecular arrays;

(ii) Advanced characterization and testing of controlled switching by state of the art scanning tunneling microscopy/spectroscopy and development of proof of concept of MFCA device.

(iii) Theoretical simulations at both the atomistic and architectural levels, transduction methodologies for input and read-out of the molecular state.

The molecular functional units should possess a strong dipolar moment, which can be oriented in either one of two opposite directions or made ineffective, whenever a perpendicular field is applied. The geometry of the self-assembled molecules determines the way they interact. The response of the molecules will be made time-variable and differentiated across space, in response to an electric field applied through a patterned dielectric layer. The project will deal to a new paradigm for device operation in which groups of molecules, in response to controlled inputs, assume the intended electric state according to the state of their neighbors. Also, a logic signals propagates under electrostatic switching to perform Boolean operation. As a proof of principle, some very basic logic state will be implemented on real molecular systems.

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Application of the Gaussian Time-Dependent Hartree Method to the Study of the Ground State of Neon Clusters

The ground state properties of neon clusters are studied through the Gaussian Time-Dependent Hartree (G-TDH) method. The presence of significant quantum effects in these systems poses a significant challenge to its theoretical investigation, because it drastically reduces the number of atoms that can be simulated in a computer. The application of the G-TDH method alleviates this difficulty, and it allows to study the ground state properties as a function of cluster size without neglecting the quantum effects. The method is based on the construction of an approximate wavefunction for the whole system, consisting in a Hartree product of normalized single-particle wavepackets of Gaussian shape. These Gaussian functions are characterized by their widths, and their centroids in position and momentum spaces. Using the Dirac-Frenkel-McLachlan variational principle and the imaginary-time propagation technique, we obtain the equations of motion that describe how these parameters approach the values that better describe the ground state of the system, and they enable to synthesize the system wavefunction of the system and to compute the structural and energetic properties of the cluster in the ground state.

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Copper – alumina composites with gradient structure

Copper-alumina composites are well known for their good frictional wear resistance, high resistance to thermal fatigue, high thermal conductivity, high absorption and dissipation of heat. The combination of properties possible in copper-alumina composites makes them particularly interesting for wear application, for example in automobile and aerospace industries.

The predominant goal of the study was to obtain a new class of alumina-copper functionally graded materials, offering technological potential for new applications such as thrusters in the aerospace industry and brake discs in the automotive industry. Because of this, the work is divided into two parts. The first part concerns composites with a low content of the ceramic phase, which can be used as thrusters, whereas the second part is focused on composites with a high amount of the alumina phase, which are expected to find application in brake discs.

The main disadvantages of composites with a low content of aluminium oxide particles include residual porosity and high internal stress generated because of differences between ceramics and metals which influence the properties of these materials. To overcome this problem aluminium oxide powder was replaced by electrocorundum. To obtain fully dense materials with a good distribution of the ceramic phase in the metal matrix, the mechanical alloying technique and Spark Plasma Sintering method were chosen. The outcome composites with the following composition: 1, 3, 5 vol. %, were analysed (microstructure and physical, thermal, tribological properties). As a result, composite materials with decreased porosity, as compared to composites reinforced with an aluminium oxide powder (α-Al2O3), were obtained. Eliminating intergranular porosity, which is undesirable from the point of view of material properties, is expected to enable manufacturing of functionally graded copper alumina composites (FGM).

For composites and functionally graded materials with a high content of the ceramic phase (i.e. >50%) an innovative technology based on pressure infiltration of liquid metal into ceramic preforms with a designed porosity gradient was developed. The technology of production of porous ceramic preforms by tape casting method of aluminium oxide foils containing a pore-forming agent, their lamination and sintering were worked out. It was shown that by controlling both amount of the added pore-forming agent and the sintering temperature of the preforms, obtaining the target open porosity in a structure is attainable. Cu-Al2O3 manufacturing procedure was based on the gas-pressure infiltration of graded porous alumina preforms by liquid copper.

The produced prototypes of a Cu-Al2O3 brake disk underwent tribological tests at the Fiat Research Centre under conditions resembling real conditions. These disks also went through a series of abrasive wear trials at different operation stages. In comparison to the reference material (i.e. grey cast iron), the obtained gradient materials are characterized by a lower degree of wear when retaining a similar coefficient of friction value due to the ceramic phase addition. Additionally, it was found that using the copper-based gradient material guarantees faster heat dissipation from the contact area.

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Eco-Friendly Nanostructured Thermoelectric Oxides for Fabrication of Miniaturized Thermoelectric Devices

In today's ever developing world, the solution for the problem that not only ensures effectively the energy production and consumption but also protects the environment is a challenge facing humanity. One of the pollution's aspects causing the warming global is the waste heat exhausted from both the energy productions and the operation of machines, equipments and vehicles like automobiles or motorbikes. The Seebeck effect-based mechanism converting heat directly into electricity of thermoelectric (TE) materials provides a promising solution that can exploit the industrial or home waste heat. Therefore, TE materials are used to fabricate the Thermo-Electric Generators (TEG). It can make the clean and green environment while implements and enriches the ways of energy production. The remarkable advances of TEGs are that they don't use heat agents originated from the fossil fuels and also don't have the moving parts like rotors in the thermodynamic motors. Thus those devices do not exhaust the toxic gases like CO2 and CO which are the cause of glass-house effect and also do not make noise considered an environment's pollution. In addition, the TE effect based energy converters are advantage and suitable to be used in rural area and for the portable devices because of their small dimension. The project aims at investigating and optimizing the fabrication parameters of novel TE thin films with nanocomposite structure based on doped ZnO and graphene oxide (GO) in order to achieve an improved power factor and decreased thermal conductivity at high temperature. For that, Sn/Co/Sb doped ZnO oxide thin films will be prepared by cost-effective methods. The overall goal is to understand the complex correlations between thermoelectric properties and structural features such as layering, orientation, dopants and lattice defects. The hybrid nanocomposite with intentionally introduced artificial nano-laminates is considered the novel mechanism that the layering may cause discontinuities in the phonon distribution and thus drastic reduction of the thermal conductivity with retained high power factor.

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Study on the modification of the fluorescence of an upconversion nanoparticle in the presence of metallic nanoparticles

The dynamical evolution of the levels of an upconversion nanoparticle co-doped with Er^3 and Yb^3 in the vicinity of a metallic nanoparticle is analyzed theoretically. A linearly polarized field with wavelength 980 nm excites the levels of the ions and produces surface plasmon resonance in the metallic nanoparticle. The effects of the interaction with the metallic nanoparticle are analyzed in dipolar aproximation. The metallic nanoparticle produces an enhacement of the local field felt by the upconversion nanoparticle increasing the upconversion efficiency. The theoretical model is compared with several experimental results to prove its validity. Finally, results of the dependence of the upconversion fluorescence with the distance between the upconversion nanoparticle and the metallic nanoparticle are obtained.

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Quantum anomalous Hall effect in stable 1T-YN2 monolayer with a large nontrivial band gap and high Chern number

The quantum anomalous Hall (QAH) effect is a topologically nontrivial phase, characterized by a non-zero Chern number and chiral edge states, which has been realized in experiment. In this work, we demonstrate the presence of QAH effect in a new stable monolayer by first-principles calculations. We show that the inclusion of SOC opens up a large nontrivial band gap of nearly 0.1 eV in its electronic band structure. The nontrivial topological properties are confirmed by the Berry curvature, anomalous Hall conductance, and the presence of chiral edge states. Remarkably, a high Chern number C = 3 is found, and there are three corresponding gapless chiral edge states emerging inside the bulk gap. Our study will enrich the family of QAH insulators.

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3-dimensional crossbar memory as the next-generation computing element

Resistance switching random access memory (ReRAM) is a highly appealing contender for a versatile replacement of NAND flash or storage class memory filling in the performance gap between dynamic random access memory (DRAM) and hard-disc (or NAND flash) in computers. Recent release of three-dimensional cross-point (3D X-point) memory jointly developed by Intel and Micron appears to be a great step-forward in this area, although the materials and process details are yet to be uncovered (ReRAM or phase change RAM). Nevertheless, main challenges in a high density three-dimensional crossbar array integration include not only the complicated vertical integration process but also the critical read/write disturbance due to the presence of sneak currents in the architecture. In this talk, feasible approaches to figure out the issues concerned to the vertical integration process, and the sneak current problem of the three-dimensional crossbar array is examined. Also, a double-layer stacked three-dimensional crossbar memory employing an extremely high performance diodecellselector is demonstrated. Beside from its ultra-high density non-volatile memory application, recent progress on the next-generation computing methods, such as the computation-in-memory and deep learning based on the emulation of synaptic learning with this memory architecture will be covered.

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Electronic and magneto-optical properties of monolayer phosphorene quantum dots

We theoretically investigate the electronic and magneto-optical properties of rectangular, hexangular, and triangular monolayer phosphorene quantum dots (MPQDs) utilizing the tight-binding method. The electronic states, density of states, electronic density distribution, and Landau levels as well as the optical absorption spectrum are calculated numerically. Our calculations show that:

(1) edge states appear in the band gap in all kinds of MPQDs regardless of their shapes and edge configurations due to the anisotropic electron hopping in monolayer phosphorene (MLP). The charge density of any edge state is only localized in specific edges of a MPQD, which is distinct from that in graphene quantum dots;

(2) the magnetic levels of MPQDs exhibit a Hofstadter-butterfly spectrum and approach the Landau levels of MLP as the magnetic field increases. A 'flat band' appears in the magneto-energy spectrum which is totally different from that of MLP;

(3) the electronic and optical properties can be tuned by the dot size, the types of boundary edges and the external magnetic field.