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PLENARY SPEAKER

Id-837

Cryogen-Free Technology for Applications in Magnetic Resonance

E. KRYUKOV*, A. KARABANOV, D. LANGLAIS, J. GOOD

Cryogenic Ltd., United Kingdom

*Corresponding author: eugeny@cryogenic.co.uk

Abstract: Magnetic Resonance (MR) is a powerful tool with many applications, including Electron Paramagnetic Resonance (EPR), Nuclear Magnetic Resonance (NMR), Magnetic Resonance Imaging (MRI) and Dynamic Nuclear Polarisation (DNP). Constantly growing problems with the cost and availability of liquid helium make limitations to the use of superconducting magnets in MR. The cryogen-free technology gives a possibility to keep the magnets in superconducting state at temperatures around 4 K without using liquid cryogens. For that a Cold Head (CH) is used, where pressure pulses of helium gas are converted into the cooling power. The high gas pressure is generated by a compressor, from which the helium gas circulates towards the CH and backwards in a closed cycle manner. A motor on the top of the CH sequentially sends the helium gas through the CH to the outlet and inlet of the compressor. Cryogen-free magnets have additional advantages over their liquid-helium counterparts. They are much more compact, because they do not require tanks to keep liquid helium and nitrogen. They do not create a dangerously high pressure and do not cause a potential risk of suffocation in case of a magnet quench. Another important innovation in cryogen-free magnets is an integrated cryostat, or Variable Temperature Insert (VTI). When the magnet reaches the base temperature, part of the cooling power from the CH can be used for cooling down the helium gas flow circulating continuously inside the integrated VTI. The temperature of helium gas, that is in a thermal contact with a sample inside VTI, can be stabilised in the range from 1.3 K up to 300 K. Magnets can be switched off for a period of time when they are not in use. A disadvantage of cryogen-free magnets is temporal magnetic field variations due to the vibrational CH operation. This restricts the use of cryogen-free technology in high-resolution NMR and MRI. Examples of application of cryogen-free magnets in EPR, NMR, MRI and DNP, its advantages and limitations will be discussed in the talk.

Keywords: Cryogen-free technology; Cold heads; Integrated VTI; Advances in Magnetic Resonance.

PLENARY SPEAKER

Id-846

Multifunctional Lanthanide-doped Oxyfluoride Nanophosphors for Luminescence Thermometry and Latent Fingerprint Detection

H. C. SWART*, G. B. NAIR, S. TAMBOLI

Department of Physics, University of the Free State, P. O. Box 339, Bloemfontein 9300, South Africa

*Corresponding author: swarthc@ufs.ac.za

Abstract: Lanthanide-doped nanophosphors have shown versatile applications across a range of sectors. In this study, lanthanide-doped oxyfluoride phosphors were synthesized via a microwave-assisted hydrothermal route and investigated for luminescence thermometry and latent fingerprint detection (LFP). LaOF:Yb^{3+},Tm^{3+} up conversion nanophosphors (UCNPs) exhibited blue and near-infrared (NIR) up conversion luminescence (UCL) under a NIR 980 nm excitation. These UCNPs exhibited temperature-dependent UCL, which was exploited for remote thermometry in the temperature range of 303 – 473 K using the fluorescence intensity ratio (FIR) technique. Meanwhile, YOF:Tb^{3+},Eu^{3+} nanophosphors demonstrated their versatility in LFP detection across multiple surfaces with complex appearances and diverse colors. With their color-tuning features, YOF:Tb^{3+},Eu^{3+} nanophosphors provided higher image contrast and higher spatial resolution of fingerprint ridges, revealing most of the details categorized as levels 1, 2, and 3. These two findings underline the potential of lanthanide-doped oxyfluoride nanophosphors as multifunctional materials for remote luminescence thermometry and high-contrast multispectral LFP detection.

Keywords: Lanthanides; Oxyfluorides; Thermometry; Latent fingerprint detection; Photoluminescence.

PLENARY SPEAKER

Id-849

Microgrippers Electro-Thermally Actuated Based Semiconductors and Polymers Materials

R. C. VOICU*, R. MULLER

National Institute for Research and Development in Microtechnologies - IMT Bucharest, 126A, Erou Iancu Nicolae Str., Bucharest-Voluntari, Romania

*Corresponding author: rodica.voicu@imt.ro

Abstract: It is well recognized that micro-electro-mechanical systems (MEMS)-based microgipper plays a vital role in micromanipulation, microrobotic and microassembly domains. In order to execute various tasks for different applications such as industry, electronic equipment's and so on, different grippers which have varied constructions composed with diverse actuators and sensors will be developed for real life [1-4]. Also, the microgrippers will be applied to not only simple jobs, but also more complex tasks since will have more degrees of freedom to provide for the requirement of varied applications. Microgrippers, as MEMS devices, are end-effectors that play an important role in the micromanipulation of biological samples (cells, bacteria, tissues), in microrobotic domain, in microassembly (MEMS/NEMS components) or in material characterization. Numerous accomplishment operations are expected for such devices, like pick-and-place, handling, grasping, releasing or manipulation of micro-elements [5-10]. In this paper, we investigate electro-thermally actuated microgrippers fabricated using silicon [8-10] and bio- polymers [2-3, 6-7], as structural materials, through surface micromachining processes. Design, simulation, characterization, and fabrication experimental tests were performed. The microgrippers were designed with V-shaped and Z-shaped electro-thermal actuators and integrated with piezoresistive force/displacement sensors for micromanipulation applications. Numerical simulations were performed in order to evaluate the behavior of the actuator and the sensitivity of the sensors as force sensor. Electro-thermo-mechanical finite-element (FEM) simulations were performed using Comsol Multiphysics software in order to analyze the performance of the MEMS devices. A comparison between the simulation results and the measurements were presented concerning the openings of the microgrippers tips. The sensitivity of the piezoresistive sensors using the electrical response of the sensors as function of displacement was numerically simulated and compared to the experimental data. A large displacement for the microgripper tips and a very small handling force for the gripper arms were demonstrated in this work. The aim of this paper is, also, to investigate the viability of silicon, as semiconductor material, with low resistivity, and epoxy resins polymers as the structural materials for microgrippers. Also, we investigated these structural materials as inexpensive materials to be used for MEMS fabrication with application in micromanipulation domains. This research was funded from the project "National Platform for Semiconductor Technologies", contract no. G 2024-85828/390008/27.11.2024, SMIS code 351364, co-funded by the European Regional Development Fund under the Program for Intelligent Growth, Digitization, and Financial Instruments and National Core Programme, Contract No 8N/2023, financed by the Romanian Ministry of Research, Innovation and Digitalization.

Keywords: Microgripper; Actuator; Electro-thermal; Sensor; Micromanipulation.

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PLENARY SPEAKER

Id-851

SERS-Based Biophotonics: From Nanotags to Microscopy and POCT

N. CHOI, E. STEPULA, V. TRAN, Y. ZHANG, S. SCHLUCKER*

Universität Duisburg-Essen, Fakultät für Chemie and Center for Nanointegration Duisburg-Essen (CENIDE), Universitätsstr. 5, D-45141 Essen, Germany

*Corresponding author: sebastian.schluecker@uni-due.de

Abstract: Surface-enhanced Raman scattering (SERS) is a highly sensitive variant of Raman spectroscopy that exploits tremendous signal enhancement from nanostructures supporting localized surface plasmon resonances (LSPRs). Molecularly functionalized gold nanoparticles, so-called SERS nanotags, can be employed as bright and photostable labelling agents for quantification and multiplexing in biophotonics. Basic considerations on the physics and chemistry of SERS nanotags, including their characterization at the single-particle level by correlative optical and electron microscopy as well as electromagnetic simulations, will be presented. Applications include immuno-SERS (iSERS) microscopy on single-cancer cells for 6-plexed bioimaging as well as point-of-care testing (POCT) with an ultrasensitive iSERS-based lateral-flow assay (LFA) employing a home-built, compact and rapid SERS reader.

Keywords: Surface-enhanced Raman scattering; Nanotags; Immunoassays; Point of care testing.

PLENARY SPEAKER

Id-853

Analyzing the Response of Intelligent Material Containing A Self-healing Agent

T. ZHELYAZOV[1,2,*]

[1]National Institute of Geophysics, Geodesy and Geography, BAS, Acad. G. Bonchev str., bl. 3, Sofia, 1113, Sofia, Bulgaria

[2]Structural Engineering and Composites Laboratory (SEL), Reykjavik University, Menntavegur 1, IS-102 Reykjavik, Iceland

[*]Corresponding author: elovar@yahoo.com

Abstract: Self-healing materials are an emerging technology that mimics the natural ability of living tissues to regenerate. They have potential applications in various fields such as dentistry, drug delivery, and construction. Given that self-healing polymer materials can also be 3D printable, they could have biomedical applications, including organ printing in the future. Researchers noticed that even non-living materials exhibit a natural capacity to regenerate under specific circumstances. For example, cracks formed in concrete can be fully or partially sealed in the presence of water. The crack sealing is mainly attributed to the continuous hydration of unhydrated cement. To enhance the capacity of man-made materials to regenerate, White et al. (2001) proposed a technique, designed to heal already formed cracks without human onsite intervention, termed autonomous self-healing. This approach presumes encapsulating a healing agent in microcapsules (with dimensions on the order of 50 μm) along with a chemical catalyst, both dispersed in the polymer matrix of an artificial composite material. The Authors presupposed a scenario in which a propagating crack breaks the microcapsules. Once released, the healing agent spreads along the crack faces by capillary action and, upon interacting with the catalyst, seals the crack. The healing agent can also be contained in: brittle containers (Li et al., 1998) (i); hollow fibers (Pang and Bond, 2005) (ii); or, alternatively, delivered by a microvascular system (Toohey et al., 2007; Mihashi et al., 2000) (iii). The healing agent can be provided in macroscopic containers embedded in the concrete (capillary tubes made of Borosilicate glass with an inner diameter of 3mm and wall thickness of 0.5 mm, Joseph et al, (2010)), or in microcapsules (with an estimated diameter of 105μm-480μm: Du et al, (2020), Li et al. (2021)). The presented contribution discusses the modeling of a material containing a self-healing agent, considering the material response at various observation scales. This is achieved by performing numerical simulations to capture damage accumulation, healing (i.e., the triggering of the encapsulated self-healing agent release), and further response of the already healed specimen. Technically, the testing protocol employed in the simulations of mechanical loading always contains three phases: an initial, pre-loading phase in which the studied specimen is damaged, but without reaching a global failure (i); a healing phase, in which the tested specimen is unloaded and the healing agent is released, and the formed cracks are fully or partially healed (ii); a second loading phase in which the healed specimen is loaded until failure (iii). Some elements of the formulation of the constitutive relationship for the material with autonomous self-healing capabilities are reported. The material model, rooted in continuum damage mechanics, is employed in some case studies; both isotropic (i.e., a scalar damage variable) and anisotropic damage (i.e., a constitutive relationship that

allows for capturing the damage-induced anisotropy in an initially homogeneous and isotropic material) are considered. Some results, reported in already published research or obtained in ongoing studies, are presented. Some results, reported in already published research or obtained in ongoing studies, are presented. Additionally, a discussion is held on some ingredients of the modeling within the representative volume element, such as the explicit description of the microcapsules and a detailed representation of the surrounding material, which are being employed in the context of an ongoing study.

Keywords: Intelligent materials; Self-healing; Damage; Modeling; Finite-element analysis.

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PLENARY SPEAKER

Id-857

Machine Learning Based Raman Spectral Analysis of Complex Biological Systems

A. KHMALADZE*

SUNY at Albany, United States

*Corresponding author: akhmaladze@albany.edu

Abstract: Raman micro-spectroscopy is widely used for chemical composition mapping within live biological samples, such as cells, organoids, and tissues. It permits non-invasive and non-destructive measurements that do not require special sample preparation processes, such as dye labelling or staining. While conventional spectral analysis techniques have been employed to extract useful patterns from Raman data, emerging developments in machine learning offer new opportunities to advance the field. In this presentation, I will discuss the applications of Raman spectroscopy to brain tissue sections, tissue engineering samples and cells exposed to iron. Through examination of spectral features in the Raman data, we detected distinct molecular bond signatures indicative of changes in key biomolecules, including proteins, lipids, and nucleic acids. We applied supervised machine learning models (Random Forest, Support Vector Machine), as well as Singular Value Decomposition to classify Raman spectra and capture patterns in the spectral data, enabling accurate differentiation between treated and control groups.

Keywords: Raman spectroscopy; Spectral analysis; Machine learning; Supervised classification; Brain tissue; Tissue engineering.

INVITED SPEAKER

Id-838

Thermal Properties of CVD Graphene by Scanning Thermal Microscopy and Finite-Elements Analysis

M. TORTELLO*, H.ZHANG, A. NAPOLITANO

Dipartimento di Scienza Applicata e Tecnologia (DISAT), Politecnico di Torino, 10129 Torino, Italy

*Corresponding author:mauro.tortello@polito.it

Abstract: Graphene and 2D materials have attracted intense research efforts, because of their exceptional electrical, thermal, and mechanical properties. The study of the thermal properties of graphene and, in general, of 2D materials, can be very relevant, for instance, for heat management of electronic circuits, given the continuous miniaturizations of the components and devices and increasing energy usage in AI and high-performance computing applications. Scanning Thermal Microscopy (SThM) [1] is a powerful tool for the thermal investigation at the nanoscale. Despite this technique hardly provides a quantitative determination of the thermal conductivity of the sample, SThM has an unmatched spatial resolution (a few tens of nanometers or less), which cannot be achieved by other popular methods such as the Raman optothermal technique or by electrical methods. We performed measurements on single layers of chemical-vapor-deposited (CVD) graphene supported by different substrates, namely, SiO_2, Al_2O_3, and PET using a double-scan technique to remove the contribution to the heat flux through the air and the cantilever [2]. By adopting a lumped-elements model, we could determine the effective properties of the supported CVD graphene layer, by modeling it as an isotropic material in *perfect* contact with the substrate and finding an effective thermal conductivity and thickness of $k_{eff} = 2.5 \pm 0.3\ \mathrm{W/m \cdot K}$ and $t_{eff} = 3.5 \pm 0.3\ \mathrm{nm}$, respectively. Despite this value might seem small for graphene, it is referred to heat flux injection perpendicular to the graphene plane. Indeed, by employing a finite-element analysis and the reported values for the perpendicular thermal conductance [3], we could provide an estimation of the in-plane thermal conductivity, k_{ab} [4], which is in good agreement with other results reported in the literature. The combination of SThM measurements and finite-elements analysis can thus be a powerful tool in the qualitative and, possibly, also quantitative analysis of the thermal properties of 2D materials.

Keywords: Scanning Thermal Microscopy; Graphene; 2D materials; Thermal properties.

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INVITED SPEAKER

Id-843

The Body in the Phage Capsid - A Detective Story

O. S. SOKOLOVA*

Lomonosov Moscow State University, 1 Leninskie gory, Bld 12, Moscow, Russia, 119234

*Corresponding author: sokolova@mail.bio.msu.ru

Abstract: Jumbo bacteriophages possess exceptionally large capsids accommodating genomes that encode additional proteins, which support their infection and replication. A distinctive structural element, known as the inner body, has been observed in a number of phiKZ-like phage particles and its proteins are believed to play an essential role in phage genome organization and ejection. However, the precise localization and three-dimensional structure of the inner body have remained elusive. Here, we applied the high-dose cryo-electron microscopy (“bubblegram”) approach to localize the inner body within the capsid of phiKZ-like jumbo phage phiK601. The inner body was resolved as a cylindrical structure approximately 22 nm in diameter, tilted by ~20° relative to the tail axis and positioned asymmetrically, likely contacting the portal vertex and the opposing capsid edge. It is surrounded by 17 concentric layers of packaged DNA and exhibits positional flexibility within the capsid. Work was supported by RSF (24-44-02003).

Keywords: Giant phage; Inner body; Bubblegrams; Cryo-EM.

INVITED SPEAKER

Id-858

DFT and Spectral Investigations of Bioactive Lanthanide Complexes

I. KOSTOVA*

Department of Chemistry, Faculty of Pharmacy, Medical University, 2 Dunav St. Sofia 1000, Bulgaria

*Corresponding author: irenakostova@yahoo.com

Abstract: Heterocyclic ligands possessing more than one donor atom, are of great interest in the field of coordination chemistry. The reason to synthesize Ln(III) complexes of biologically active coumarin derivatives was to compare and find out the differences between known and the new Ln(III) complexes with other bioactive ligands. It is expected that the complexes will retain or improve the activity of the initial organic ligands. The synthesis of Ln(III) complexes is taken into consideration with the study of their cytotoxic and antioxidant effects. The molecular quantities as: vertical ionization potential, electron affinity, electronegativity, hardness, electrophilicity indices, Fukui functions, molecular electrostatic potential of the neutral and double deprotonated species were calculated and discussed to suggest the most probable binding sites and to obtain the optimized geometries of the studied compounds. A range of analytical and spectroscopic methods have been applied (elemental analyses, mass-spectra, ^{1}H NMR and ^{13}C NMR spectra, FTIR and Raman spectra, as well as UV-VIS spectral analysis). The DFT results showed the most probable reactive sites for electrophilic attack. The data of IR, Raman, UV-VIS and NMR spectra confirmed that the theoretically suggested donor atoms were involved in the coordination to the metal ions. Further, molecular modelling was performed to obtain the most probable molecular geometry of the obtained Ln(III) coordination compounds. The DFT was found as a reliable method for calculations of geometries and vibrational frequencies of the compounds. The results of the cytotoxicity screening and antioxidant activity have shown that in contrast to the observed effects of the Ln(III) complexes, the corresponding nitrates were practically devoid of cytotoxicity and antioxidant properties at the same experimental conditions. This research provides a starting point for a series of new coordination compounds that have not been tested before for antitumor and antioxidant properties. The administrative support received by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project No. BG-RRP-2.004-0004-C01 is greatly acknowledged.

Keywords: Metal-based compounds; Theoretical; Analytical; Spectroscopic; Cytotoxicity; Antioxidant activity.

POSTER PRESENTATION

Id-576

Lateral Flow Immunoassay of Beta-Agonist Mabuterol using Au@Ce Nanoparticles as A Signal-Enhancing Label

E. A. ZVEREVA*, P. S. LUKINA, V. G. PANFEROV, O. D. HENDRICKSON, A. V. ZHERDEV, B. B. DZANTIEV

A. N. Bach Institute of Biochemistry, Research Center of Biotechnology of the Russian Academy of Sciences, Moscow, Russia

*Corresponding author: zverevaea@yandex.ru

Abstract: Growth promoters, particularly beta-adrenergic agonists (beta-agonists), are widely used to enhance livestock production. Beta-agonists stimulate specific receptors in the muscle tissue of farm animals, increasing fat conversion and synthesis of skeletal muscle proteins, and by this way - leading to muscle growth. However, beta-agonists consumed through food disrupt different metabolic processes and have negative impact on human health. This necessitates rapid testing of food products for beta-agonists. The lateral flow immunoassay (LFIA) provides an effective methodological solution for this purpose due to rapid analytical procedure and simple interpretation of results.An immunoassay for the beta-agonist mabuterol (MAB) has been developed using indirect labeling via a conjugate of gold nanoparticles (AuNPs) with anti-species antibodies. The development of the LFIA included optimization of the immunoreagent concentrations and the reaction mixture composition (buffer type and pH, ionic strength, detergents). The reached instrumental detection limit was 1.6 ng/mL. The analysis duration was 15 min. Novel bimetallic Au@Ce nanoparticles (Au@Ce NPs) were synthesized and characterized as alternate labels for LFIA. The peroxidase-like properties of Au@Ce NPs allowed for catalytic amplification of the optical signal on the test strips, increasing the sensitivity of the analysis. The proposed enhanced assay demonstrated instrumental detection limit equal to 0.3 ng/mL. The analysis duration was 18 min, which included a three-minute incubation with the substrate solution (3,3',5,5'-tetramethylbenzidine, H_2O_2, and dextran sulfate). The efficiency of the developed LFIA method for detecting medical agents in raw meat samples was demonstrated. The obtained results confirm significant potential of the developed test systems as effective tools for mass monitoring of beta-agonists in food products. This study was funded by the Russian Science Foundation (project 25-16-00214).

Keywords: Meat products; Beta-Agonist; Food safety; Lateral flow immunoassays; Au@Ce nanoparticles.

POSTER PRESENTATION

Id-585

Advanced Bioactive Textile Systems with Enhanced Antibacterial Performance for the Management of Post-Traumatic Skin Infections

M. F. DONDEA*, E. VISILEANU, A. F. VLADU, R. R. CONSTANTINESCU

The National Research and Development Institute for Textiles and Leather,

16, Lucretiu Patrascanu,sector III, code 030508 Bucharest, Romania

*Corresponding author: felicia.dondea@incdtp.ro

Abstract: In this study, two knitted textile substrates with compositions of 80% cotton / 20% elastane and 45% cotton /55% polyester were used. These materials were treated with active substances in order to impart antibacterial properties. The study was structured around three treatment variants, based on different substances with antibacterial potential. The first variant involved the use of a mixture of pine, eucalyptus, and rosemary essential oils, together with sodium alginate, which acted as a fixing agent on the textile substrate. The second variant included collagen, collagen combined with a colloidal silver solution, and chitosan with colloidal silver, substances known for their antibacterial activity and biocompatibility. The third variant focused on the microencapsulation of pine essential oil, using collagen, zeolite, and β-cyclodextrin, with the aim of improving the stability of the active substance and ensuring its controlled release. The antibacterial evaluation was performed using strains of *Escherichia coli*, *Staphylococcus aureus*, and *Candida albicans*. The results demonstrated a satisfactory antibacterial effect for all tested samples, as no bacterial growth was observed following the incubation period. This absence of microbial proliferation indicates that the applied treatments were effective in inhibiting the growth of *Escherichia coli*, *Staphylococcus aureus*, and *Candida albicans*. The findings confirm the antibacterial potential of the active substances used, regardless of the textile substrate composition, and highlight their suitability for application in textile materials intended for medical or post-traumatic skin infections use. This work was carried out through the Core Programme within the National Research Development and Innovation Plan 2022-2027, carried out with the support of MEC-ANC, project no. 6N/2023/PN23260201/2300001.7 project title "Intelligent equipment to ensure combatant survival in operational conditions'' IRHEM.

Keywords: Essential oils; Bioactive substances; Textile materials; Antibacterial effect; Wound healing.

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POSTER PRESENTATION

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Investigations on the Structural and Morphological Evolution of LSC Nanofibers

E. Ç. KONUKCU, O. A. AKSAN*, N. KIZILDAĞ

Gebze Technical University, Institute of Nanotechnology, 41400, Kocaeli/Türkiye

*Corresponding author: oaksan@gtu.edu.tr

Abstract: Perovskite nanofibers represent a compelling class of functional materials that combine the high surface area and anisotropic morphology of one-dimensional nanostructures with the remarkable electronic and catalytic properties of perovskite oxides. Their morphology and crystal structure are governed by the combined influence of electrospinning parameters and subsequent calcination conditions. In this study, lanthanum strontium cobaltite ($La_{0.6}Sr_{0.4}CoO_3$, LSC) nanofibers were synthesized via electrospinning followed by calcination to systematically investigate the effects of processing parameters on their structural and morphological evolution. Polyacrylonitrile (PAN) was employed as a carrier polymer at varying concentrations to obtain homogeneous PAN–LSC composite nanofibers. The as-spun composite fibers were calcined at 700 and 800 °C to remove the polymer matrix and promote the formation of the perovskite oxide phase. Scanning electron microscopy (SEM) was used to analyze the post-calcination morphology and fiber diameter distribution, while X-ray diffraction (XRD) was performed to evaluate phase formation and crystallinity. SEM results demonstrated that the fibrous morphology was largely preserved after calcination, whereas XRD patterns revealed a progressive transformation from an amorphous precursor to a well-defined crystalline perovskite phase with increasing calcination temperature. This study was supported by Scientific and Technological Research Council of Turkey (TUBITAK) under the Grant Number 124M101. The authors thank to TUBITAK for their supports.

Keywords: Electrospinning; Nanofibers; Perovskites.

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