Any sufficiently advanced technology is equivalent to magic

Sir Arthur C. Clarke

1st external seminar of the Plasma Chemical Technologies Department

(Head: Dr. Maksym Buryi)

Plasma chemical technologies as the important approach to the (nano)materials and hydrogen production

Editor: Dr. Maksym Buryi

Marianská, Czech Republic
10-12. 06. 2024
Foreword

The seminar is dedicated to the main activities of the Plasma Chemical Technologies Department, Institute of Plasma Physics of the Czech Academy of Sciences with respect to the national and international R&D. In particular, the advanced methods of the (nano)materials synthesis, fabrication and characterization as well as in many cases green hydrogen production will be presented and discussed in detail. The aim of the seminar is to establish more of the effective paths of communication and data exchange by creating and maintaining links among the teams of national and international experts in various fields. These include physical and chemical knowledge, both experimental and theoretical, with an accent put on plasma, as well as to create a bridge to commercialization of scientific findings and technology transfer. In addition, the connection to the medical, biological, ecological sciences and materials engineering is provided. This will in turn create the basis for the synergy of science and industry to pave the way for the wider collaboration with the world-wide experts engaged in pure research and production of different materials of any form (in particular, hydrogen, carbon nanoparticles and other nanomaterials). In this respect, it is appropriate to mention that the expected outcome is hydrogen production as well as new materials design by applying the set of experimental and theoretical techniques and methods. Among the others, plasma chemical technologies including computational fluid dynamics, physics and techniques of microwaves, electron paramagnetic resonance, and first principles calculations can be mentioned. Their combination complemented with the other experimental methods is the strongest tool giving feedback to any technology, thus leading to the desired material synthesis and fabrication. The expected practical outcomes finding implementation in industry are various sensors, sorbents, light emitting devices, protective layers, energy to X and X to energy concepts etc. Therefore, the importance of the meeting can hardly be underestimated. We believe that this first external seminar of the department will continue becoming annual stretching out the ideas of national and international collaboration for the improved R&D.

The organizing committee consists of Dr. Maksym Buryi (Head), Dr. Alan Mašláni (Deputy), Dr. Michal Hlína and two Ph.D. students Jakub Pilař and Ondřej Šot (further mentioned in the text as “Committee”). The financial support of this networking event from the program “Strategy AV 21” of the Czech Academy of Sciences, specifically work package VP 27 (Efficient energy transformation and storage) led by Dr. Alan Mašláni, is gratefully acknowledged. Further, the Committee would like to express deepest gratitude to the external national and international experts for their active participation: Prof. Bohuslav Rezek from Czech Technical University, Prof. Michał Piasecki from the Jan Długosz University, Prof. Mauro Fasoli from the Milano-Bicocca University and Dr. Tomáš Mates from the HVM Plasma Ltd.
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Plasma Chemical Technologies Department

Institute of Plasma Physics of the Czech Academy of Sciences


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Fields of interest. Scientific and commercial/industrial relevance

Capabilities of the Department. Cooperation offer

O1. Synthesis gas (syngas) of the (100-x)%H$_2$ + x%CO (x = 10-50) production out of any kind of organic input materials (hydrocarbons) including but not restricted to gases (e.g., methane, biomethane, natural gas etc.), liquids (e.g., oil), solid phase (any kind of plastics, pure, such as polyethylene, polypropylene etc., and mixed like the plastics from electronic devices; refused derived fuel (RDF); wood, paper, cellulose, lignin etc.; sewage sludge; agricultural waste etc.) using thermal plasma gasification/pyrolysis. The amount is about 40-50 kg/hour.

O2. Carbon nanoparticles (graphite, graphene) production of different geometry (ball-shape (also porous), nanotubes (single and multi-wall ones)) at the kilograms scale applying thermal plasma gasification/pyrolysis to the input materials from the point 1. Physical (plasma treatment, annealing etc.) and chemical (etching, growth of carbon or other nanoparticles and quantum dots to create heterostructures) modifications for various applications. The amount is at the level of kilograms to tens of kilograms per day.

O3. Application of thermal plasma gasification/pyrolysis to any kind of inorganic input materials (e.g., crystals, ceramics, glass etc.) to produce nanoparticles at the level of kilograms per day.

O4. Modelling and calculation of plasma properties using computational fluid dynamics, thermodynamic equilibrium, energetic and economic balances including: modelling of gasification of solid organic/inorganic waste using arc plasma torches; physics and modelling of electric arcs; calculation of thermodynamic functions; determination of molecular data; composition of complex systems.

O5. Experimental characterization of gases as well as nanoparticles including mass spectrometry, chromatography, luminescence and magnetic resonance data interpretation.

Search for cooperation

S1. Input materials providers (organic and inorganic) for utilization and valorisation to syngas/hydrogen and/or nanoparticles of any kind.

S2. Purification of syngas from dangerous gases – byproducts of the plasma gasification such as HCl, H$_2$S, NO etc.


S4. Realization of produced: (i) purified syngas; (ii) separated H$_2$ and CO (points S1,2); (iii) carbon (graphite, graphene) and non-carbon nanoparticles (any kind, e.g., metals or metal oxides, halides etc.) including heterostructures.

Academic cooperation with higher education

There are five Ph.D. students currently employed at the department in cooperation with Czech universities such as University of Chemistry and Technology in Prague, Czech Technical University and University of Pardubice under the (co-)supervision of the department senior scientists. We are open also for further pedagogical cooperation.

Equipment

4
Reactor PlasGas (200 litters volume)
Our flagship reactor, built in 2004 in cooperation with industrial partners from Belgium and from the Czech Republic. The reactor is continually upgraded to cope with new projects. The internal refractory lining is able to withstand temperatures up to 1500 °C and there is a possibility to dose wide variety of solid, liquid and gaseous fuels or materials to be treated. So far, we performed experimental research of plasma gasification, pyrolysis and reforming of wood, sawdust, pellets, lignite, waste plastics, polyethylene, polypropylene, simulated medical waste, refused derived fuel (RDF), pyrolytic oil, methane, simulated natural gas and ethanol. The produced gas is sampled directly at the output of the reactor and then can be cooled to a desired temperature by water spray system. The reactor is maintained at slight underpressure by a powerful water ejector system. The gas is then safely combusted in a flare.

Kinetic reactor
Reactor specially designed for the study of the kinetics of the gasification, reforming and pyrolysis processes taking place along the axis of the reactor. Reactor is smaller than PlasGas reactor and it is equipped by the special air/water/argon plasma torch with lower power.
Low-pressure reactor
Designed to study the effect of ambient pressure on arc characteristics and jet properties, to study the supersonic jet with extremely low plasma pressure and to investigate the utilization of supersonic jets for plasma chemical applications and for plasma spraying.

WSP-H – so called hybrid WSP (Water Stabilized Plasma) torch
In the WSP-H torch, plasma is formed by electric arc from water steam and gas (argon). This approach combines benefits of gas stabilization (non-consumable tungsten cathode) and water stabilization (high enthalpy). Application of water as a plasma forming medium, together with its high enthalpy, brings apparent advantages for gasification and pyrolysis, in comparison with commonly used air plasma. The latest generation of WSP-H torches was developed in cooperation of our institute and ProjectSoft HK a.s. company. Input power up to 160 kW can be applied. This torch is also successfully used for plasma spraying (see https://www.wsp-h.com/ and site of Department of Material Engineering http://www.ipp.cas.cz/vedecka_struktura_ufp/materialove-inzenyrstvi/)

Microwave plasma torch
This new torch with power up to 75 kW is currently installed in our laboratory. It is supposed to be used for gasification and pyrolysis applications, especially for gases, e.g., methane. Nitrogen fixation is also realized.

Steam plasma torch
The plasma torch TransCut 300 was developed by Fronius International GmbH, Austria. The liquid mixture of water and ethanol is heated and produced vapour is used as a plasma forming gas. This torch was originally designed for plasma arc cutting. It has input power up to 5 kW, i.e. much lower than WSP-H. We use it for demonstration of steam arc plasma technology and for testing the plasma chemical processes in small scales.
**Diagnostic**
- High-speed camera Photron FASTCAM SA-X2 with maximum frame rate 1080 000 fps and minimum exposure time 0.25 µs; the camera is synchronized with the Cavilux HF laser with wavelength 810 ± 10 nm; the pulse power of the laser is up to 500 W and the pulse duration can be varied between 50 ns and 10 µs – study of fast processes connected with plasma and its interaction with particles of treated material can be performed.
- Optical spectrometer Triax 552 equipped with gratings 300, 1200 and 3600 grooves/mm giving spectral resolutions 0.16 nm/pixel, 0.036 nm/pixel and 0.0098 nm/pixel respectively. The output spectrum is detected by the iCCD detector with 1024x256 pixels.
- Optical spectrometer Flame - Ocean Optics for low resolution overview emission spectra in the range 200-1100 nm
- Quadruple mass spectrometer – online gas and plasma sampling in various positions in reactor volume and determination of local composition of plasma and gas.
- FT-IR spectrometer Matrix – concentration measurement of output gases
- Enthalpy probe Tekna connected to quadruple mass spectrometer – measurement of plasma enthalpy, temperature, composition and flow velocity in the positions where heat flux does not exceed limiting values for probe destruction.
- Borescope camera with gas flow protection of optics – allows optical insight into the hot and chemically active environment in reactors.

**Selected relevant ongoing projects**

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<th>Project ID</th>
<th>Provider</th>
</tr>
</thead>
<tbody>
<tr>
<td>NCK MATCA II (National centre of competence for Materials, Advanced Technologies, Coatings and their Applications) (Mgr. Alan Mašláni, Ph.D.)</td>
<td>TN02000069</td>
<td>TA CR</td>
</tr>
<tr>
<td>Membrane separation of carbon dioxide from flue gas and its subsequent use (Mgr. Alan Mašláni, Ph.D.)</td>
<td>TK02030155</td>
<td>TA CR</td>
</tr>
<tr>
<td>Center of Energy and Environmental Technologies (CEET) (Ing. Jiří Jeništa, CSc.)</td>
<td>TK03020027</td>
<td>TA CR</td>
</tr>
<tr>
<td>Advanced Confined CsPbBr₃/ZnO/PS Nanocomposite Structure With Efficient Response to Ionizing Radiation (ANSWER) (Mgr. Maksym Buryi, Ph.D.)</td>
<td>24-12872S</td>
<td>CSF</td>
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Imperfection, Low-Dimensionality and Tensioning as the Efficient Ways to Improve the Desired Properties of Materials

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Is well known that the stress or strain influents on structural, optical, magnetic, electrical or superconducting properties of solids. Recently has been spectacularly demonstrated that lattice mismatch between thin films and/or substrate gives an extraordinary opportunity for materials engineering. Thanks to these phenomena, newly constructed (transformed) materials, possess totally different properties, than are desired in nature. Especially, two-dimensional systems are ubiquitous in today technology and condensed matter physics. The physical laws of ordinary matter are prone to be radically modified by reducing the dimensionality, and completely new phenomena can manifest themselves. The strain imposed by the substrate onto which the films are epitaxially grown provides extra degrees of freedom to tune the behavior of the films. Strain caused by external pressure or temperature changes can influence on the transition temperatures, induce phase changes and modify the symmetry of the films. The symmetry differences usually bring important changes in the functional properties (polarization, dielectric permittivity, piezoelectric response, emission properties etc.), which are highly anisotropic. We will demonstrate that a single experimental parameter, strain, simultaneously controls multiple order parameters and is a viable alternative tuning parameter to composition modification.

Later in the lecture we will focus on the influence of composition (and its imperfection), size, temperature or pressure on the structure, electronic and luminescence properties. Finally, examples improved (or tuned) promising materials interesting for superconductivity, dosimetry, remotely temperature and pressure sensing will be discussed.
Interactions of molecules with semiconductor surfaces have always been a crucial topic in physics, chemistry, and materials science due to the novel and interesting structural, chemical, electronic, and optical properties of such interfaces [1]. However, there are still large gaps in understanding the interfaces between metal oxide semiconductors and biomolecules (from proteins to single amino acids).

Therefore, to provide a better insight and interpretation of data in the literature [1,2], we have focused in our work on computational and microscopic study of interactions between the ZnO surfaces and two well-known and biologically important molecules, bovine serum albumin (BSA) and thiorphan. We compare the adsorption of these molecules on different ZnO polar and non-polar surfaces, investigated the role of surface chemistry and surface dipole magnitude and orientation. The classical force field method and quantum-based density functional tight binding (DFTB) approaches are employed in a complementary manner. The computational findings are complemented by atomic force microscopy (AFM) measurements in various regimes.

The results of simulations and AFM show that BSA adsorbs on all the studied ZnO surfaces while specific interaction and arrangement are considerably affected by the atomic surface structure of ZnO [3]. In the case of thiorphan, molecular dynamics simulations using CO dipole arrays to mimic ZnO surface polarity show that the surface polarity, giving rise to different electric field orientation and magnitude, has the key role in molecular assembly observed by AFM (from nanodots to nanolayers) rather than the surface chemistry [4]. Study of biomolecules interacting with magnetized surfaces shows also interesting dependency on direction of magnetic dipole. The results may be helpful for designing and understanding function of ZnO-based materials in various applications ranging from biomedicine and biosensing to optoelectronics and spintronics.

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References
Thermoluminescence as a Tool for Investigating Defects in Luminescent Materials

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Thermally Stimulated Luminescence (TSL) technique, often referred to just as thermoluminescence, has been extensively employed in various applications where the estimation of the dose delivered to a material is required. These applications include various types of dosimetry (personal, environmental, retrospective, accident, etc.) and dating of ancient artifact such as pottery, clays, etc.

However, TSL has shown to be extremely useful also in the investigation of defects in luminescent materials. In fact, the signal registered during a TSL measurement is due to the radiative recombination of charges released from localized point defects, which act as trapping sites during exposure to ionizing radiation. The information that can be obtained by analyzing TSL data is particularly important for scintillators where trapping sites play a critical role in the performances of the material. In fact, depending on their stability (e.g. decay time) traps can either reduce the scintillator light yield or produce slow components in the scintillation emission because of delayed recombinations.

In this presentation, a short introduction to the basic principle of TSL will be provided together with some examples of the potentiality of the technique applied to various types of luminescent materials. Moreover the importance of coupling TSL to other spectroscopic techniques, Electron Paramagnetic Resonance (EPR) in particular will be described.
Humanity is surrounded by microwaves appearing in, practically, all aspects of our lives. This is a very specific kind of electromagnetic waves with the frequencies ranging from 0.3 to 300 GHz. The most important kinds of microwaves in-house applications commonly known among customers are (the specific frequencies are given in parentheses): cell phones (about 900 MHz), microwave ovens (2.45 GHz), satellite antennas and phones, radars (about 1 GHz-300 GHz), microwave plasma torches (915 MHz, 2.45 GHz) etc. Only microwaves are able to pierce the ionosphere of Earth and only due to them there is the possibility of communication between Earth and e.g., International Space Station. Spreading of the microwaves has a peculiarity as it depends on the type of oscillations known as mode. There are three of them: TE (transversal electric field, i.e., the electric field component along the direction of the electromagnetic wave propagation is missing), TM (transversal magnetic field, i.e., the magnetic field component along the direction of the electromagnetic wave propagation is missing) and TEM (transversal electric and magnetic field, i.e., the electric and magnetic field components along the direction of the electromagnetic wave propagation are missing). TE and TM are spreading only inside the rectangular or cylindric waveguide whereas the TEM can appear in coaxial waveguide (like the known antenna cable) and open space. The TE and TM modes depend on the geometry. Schematically, the propagation of microwaves (the distribution of the electric and magnetic fields inside a rectangular waveguide) is shown in Fig. 1 on example of the TE_{01} mode.

Fig. 1. Spreading of the microwaves of the TE_{01} mode inside a rectangular waveguide. Different directions are considered.
Electron Paramagnetic Resonance in Gases

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In contrast to those in condensed phases, atoms and molecules observed in the gas phase are nearly entirely free to execute translational motion. There are no direct spectroscopic repercussions because such motion (i.e., of the species center of mass) does not create any detectable energy splitting. However, quantized rotational energy levels can be observed through literally free molecule rotation; these splittings are frequently the same as those of the Zeeman spin states. The rotation-magnetic interactions that follow have a significant impact on diatomic and polyatomic molecules' EPR spectra.

For gas-phase systems, angular momenta continue to be important if comprehension of the EPR transitions is to be achieved. These originate from four sources: nuclear spin(s), rotation of the nuclear framework, and electronic (total) orbital motion and spin. Here, it can be assumed that the set of total angular momentum vectors of the atoms or molecules is randomly oriented, but each remains locked in its orientation until a collision occurs, which is, in most studies, a rather rare event on the EPR time scale. Actually, it is not possible to measure the quantum number until an external magnetic field is introduced, or, more precisely, until a quantization direction is determined.

Relaxation times and linewidths may be significantly impacted by collisions with the container walls or between atoms and molecules. There are literally no electrically charged species that have been detected in the gas phase by EPR primarily due to the inability to get large enough ion concentrations for conventional EPR investigations. A paramagnetic gas phase sample's observed line positions and multiplicity in the EPR spectrometer provide precise information about a variety of intriguing molecular characteristics.

Moreover, investigations of reaction kinetics as a function of time can be made. The focus is mostly on species that have one or more unpaired electrons, e.g., appearing in doublet and triplet states. Interestingly, EPR spectra can also be obtained from species that lack net electron spin but display electronic orbital magnetism.

Acknowledgements. This work was supported by the Funding Organization project No. 27012400.

References
[2] Lok Yiu Wu, Chloé Miossec and Brianna R. Heazlewood, Chemical Communications. Issue 20, 2022
Chromatography

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Chromatography, first devised at the University of Kazan by the Italian-born Russian botanist Mikhail Tsvet in 1900 [1], is an analytical and preparative technique widely used for the separation of mixtures into their individual components. This process involves a system where the analyte travels through a stationary phase while being carried by a mobile phase. The mobile phase can be a gas or a liquid, leading to different types of chromatography such as gas chromatography (GC) and liquid chromatography (LC).

In chromatography, the stationary phase may be housed in different formats including capillaries, columns, plates, or sheets. The analyte's interaction with both the stationary and mobile phases facilitates its separation based on different physical and chemical properties. Detection and collection of the separated components are crucial steps in the process, typically achieved through various types of detectors that provide identification and quantitation.

In gas chromatography, the Flame Ionization Detector (FID) is widely used for organic compounds, detecting ions produced during the combustion of analytes in a H₂ flame. The Thermal Conductivity Detector (TCD) measures changes in the thermal conductivity of the gas stream, suitable for a wide range of compounds, including inorganic gases. The Electron Capture Detector (ECD) is highly sensitive for halogenated compounds, detecting those that can capture electrons.

Liquid chromatography, particularly high-performance liquid chromatography (HPLC), often employs detectors like the Ultraviolet-Visible (UV-Vis) detector, which measures the absorbance of light by sample components, and the Diode Array Detector (DAD), which provides a full spectrum for each peak using multiple wavelengths. The Fluorescence Detector (FLD) is highly sensitive for naturally fluorescent compounds or those that can be derivatized to fluoresce, while the Refractive Index Detector (RID) measures changes in the refractive index of the eluent, useful for compounds with low UV absorbance.

Chromatography is pivotal in numerous fields such as food analysis (for carbohydrates, proteins, vitamins, etc.), pharmaceutical analysis (impurity analysis, degradation monitoring), environmental monitoring (measuring air pollution), and forensics (blood alcohol analysis). It is also critical in the petrochemical industry for analyzing polymers, solvents, and other products. Preparative chromatography is important in organic chemistry for the purification of substances on an industrial scale.

References

Optical emission spectroscopy of thermal plasma for plasma chemical applications

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Thermal plasmas generated by arc discharge in plasma torches can reach temperatures more than ten thousand of Kelvins. Experimental determination of plasma composition and temperatures in such conditions is possible more or less only using the emitted radiation. This radiation is strongest in the spectral ranges from ultraviolet through visible up to infrared. Accuracy of measurement is substantially increased if radiation can be split into the spectrum with the highest possible spectral resolution. In such case we can analyse radiation in individual wavelengths, which consists of continuum component and discrete spectral lines corresponding to ions, atoms and molecules in plasma. Except high spectral resolution also high spatial resolution of measurement is often required. In such case the problem of high temperature gradients between central parts of arc column and plasma edge must be solved, since the measured radiation contains contributions from these different regions. Problem becomes even more complicated in case of interaction of plasma with solid, liquid or gaseous materials. Such an interaction takes place in open air (e.g. plasma arc cutting) or in the reactors for pyrolysis and reforming of organic components, which are operated by IPP. The ultimate goal is destruction of unwanted waste materials and/or production of synthesis gas, hydrogen or high-quality carbonaceous material. In this contribution, the short summary of optical emission spectroscopy diagnostics applied to thermal plasmas in various conditions will be presented.

Acknowledgements. This work was supported by the Academic Research Agency AV 21 under the program Efficient energy transformation and storage
Thin films are a special area of materials engineering that elegantly expand the application area of various components by fundamentally improving the properties of the substrate. Their function can be mechanical, optical, decorative (aesthetic) or other (combined). Their utilization in automotive industry can significantly improve the efficiency or lifetime of some components [1,2]. We will provide a brief overview of the methods, which are used for the thin film preparation and characterization. The main part will be devoted to selected case studies of both tribological layers [3] (used for mechanical protection of components) and decorative layers [4] (fulfilling special appearance requirements with added mechanical protection). The concept of the multilayer structure will be explained and demonstrated by some examples. We will also show microscopy images of layer defects [5] and discuss the ways of their treatment either via adjusted process parameters or substrate inspection and modification. Finally, we summarize the basic facts about thin films, their properties and applications.

Fig. 1. (a) Examples of thin film application areas in the automotive. (b) Example of a protective thin films with a multilayer structure. (c) Study of the growth defects in the tribological W-C:H multilayer.

Acknowledgements: This work was funded by the HVM Plasma, spol. s r.o. within the internal project PR17_29_06 Growth defects and by the MEYS CR Projects LM2015087, LM2018110 and LM2023051.

References
Illuminating the Future: The Multifaceted World of Carbon Dots in Science and Technology

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Carbon quantum dots, commonly referred to as C-dots, are a fascinating category of carbon-based nanoparticles that have garnered significant scientific interest. This is primarily due to their unique ability to emit light (photoluminescence), coupled with their abundance, cost-effectiveness, and non-toxic nature [1]. These nanoparticles are distinguished by their exceptionally small size, which typically measures less than 10 nanometers, their remarkable stability when exposed to light, and their impressive biocompatibility, making them well-suited for interactions with living organisms[2].

The intriguing properties of carbon dots, such as their robust light-emitting capabilities, high chemical stability, and ease of functionalization, have paved the way for their application in a variety of advanced fields. These applications span from biomedical imaging and fluorescent labeling to acting as catalysts in light-driven chemical reactions and contributing to environmental remediation efforts [3].

In this seminar, we will delve deeply into several key aspects of carbon dots. First, we will explore the various synthetic methods used to create these nanoparticles. These methods include top-down approaches like laser ablation and arc discharge, as well as bottom-up techniques such as hydrothermal/solvothermal synthesis, microwave synthesis, and electrochemical methods. Each synthesis method offers unique advantages and potential drawbacks, influencing the resulting properties of the carbon dots.

Next, we will examine the diverse properties of carbon dots that make them so versatile. This includes their optical properties, such as excitation-dependent emission, quantum yield, and photostability. We will also discuss their chemical properties, including surface functional groups that can be tailored for specific applications, and their physical properties like size distribution and shape.

The seminar will then highlight the wide range of applications for carbon dots. In biomedical imaging, carbon dots serve as fluorescent probes due to their bright and stable emission, aiding in cellular imaging and diagnostic techniques. As sensors, they can detect various biomolecules and environmental pollutants with high sensitivity and specificity. Additionally, in light-driven chemical reactions, carbon dots can act as photocatalysts, facilitating processes such as water splitting and pollutant degradation.

By the end of this seminar, attendees will have a comprehensive understanding of how carbon dots are synthesized, their unique properties, and their vast potential in various scientific and industrial fields. Moreover, we will underscore the importance of ongoing research to fully harness the capabilities of these remarkable nanoparticles.

References


Nickel-Carbon Composite Nanomaterial Synthesis via Plasma Catalytic Pyrolysis

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The experiment was conducted using the PLASGAS plasma reactor, which has an internal volume of 200 liters and utilizes the Hybrid Water Stabilized Plasma torch. The characteristics of the Hybrid Water/Gas DC Arc Plasma Torch and the PLASGAS reactor are detailed by Hrabovský et al. [1] and Fathi et al. [2], respectively. Previously, this system has been employed for the pyrolysis of methane [3] and natural gas [4]. In this study, however, we investigate methane pyrolysis by adding Nickel Oxide powder as a catalyst.

This experiment introduced a 100 SLM methane feed into the reactor, with plasma power set at 110 kW. The resulting gas composition was 86.5 vol\% hydrogen and 12.1 vol\% carbon monoxide, with only 1.2 vol\% methane remaining unconverted and 0.1 vol\% acetylene produced. In addition to hydrogen production, a solid carbon-nickel (core-shell) structure nanocomposite material was synthesized. XRD and EDX analysis confirmed that the nickel oxide was reduced to zero-valent nickel nanoparticles with particle sizes less than 50 nm. The TEM images of the produced composite material are shown below.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{TEM_images.png}
\caption{HRTEM images.}
\end{figure}

References


Phosphate Glasses and Their Use as a Matrix for the Creation of Glass Ceramics

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Phosphate glasses, characterized by their unique network structure of PO$_4$ tetrahedra, exhibit distinct properties such as low melting temperatures, high thermal expansion coefficients, and good solubility for various metal oxides. These attributes make them promising candidates for glass ceramics, a versatile class of materials formed by controlled crystallization of glass. The potential applications of phosphate-based glass ceramics are broad, spanning biomedical fields due to their bioactivity and biocompatibility, to optical and electronic devices owing to their tunable refractive indices and electrical properties. Ongoing research focuses on optimizing parent glass matrix and controllable reproducible synthesis to enhance their performance and extend their use in advanced technological applications. In current research, we focus on the incorporation of metal halide perovskite materials from the CsPbBr$_3$ family into phosphate glasses.

The combination of CsPbBr$_3$ and phosphate glasses in the development of glass ceramics is an area of significant interest due to the unique and complementary properties of these materials. CsPbBr$_3$, a perovskite compound, is known for its exceptional optoelectronic properties, including high photoluminescence quantum yields, tunable emission wavelengths, and excellent charge carrier mobility. Integrating CsPbBr$_3$ into phosphate glasses to form glass ceramics can enhance these properties while benefiting from the structural and thermal advantages of the glass matrix.

Phosphate glasses serve as an excellent host material due to their low melting points, high thermal expansion coefficients, and good solubility for various metal oxides, including those used in perovskite compositions. The incorporation of CsPbBr$_3$ into phosphate glass matrices through controlled crystallization can lead to the formation of nanocrystals within the glass, creating a composite material that combines the mechanical and chemical stability of the glass with the superior optoelectronic properties of the perovskite nanocrystals.
A macroscopic description of a system as given by experimental observation is possible to model by a
dynamical system of interacting particles following laws of classical or quantum physics. Although the
Hamiltonian representing the many-body problem is not separable it is still possible to find plausible
approximations by separation of molecular internal degrees of freedom and coordinates of center of
mass to factorize phase space. The dimensionality of many-body system in quantum mechanics scales
exponentially contrary to linear scaling of classical phase space system. The assumption of the molecular
and gas space allows under given constraints as follows e.g. from spatial symmetry or fixed positions of
nuclei in crystal lattice to reduce dimensionality of the problem. Molecular dynamics describes many-
body problem via solution of equations of motion while statistical mechanics replace lack of information
on a system by laws of statistics. Both approaches, however, consider interaction of molecules, nano-
particles or lattices of a solid phase material, which follows laws of quantum mechanics. Description of
these microscopic objects of chemical interest by methods of molecular quantum mechanics is subject
of quantum chemistry. *Ab initio* methods in quantum chemistry traditional starts from Hartree-Fock
(HF) self-consistent field (SCF) in Born-Oppenheimer approximation (BO) [1]. Nowadays, vibronic
coupling as effect beyond BO, in photochemical induced reactions is of increasing importance [2].
Correlation of electrons due to coulomb repulsion by truncated linear configuration interaction (CI) as
CISD is generally incapable to conserve size extensivity. This problem size-extensivity in correlation is
solved by exponential ansatz and Hausdorff expansion in coupled cluster methods [3].

References

Modelling of Gasification of Crushed wood in Thermal-plasma Chemical Reactor

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The lecture presents numerical simulation of gasification of crushed wood using a unique plasma torch stabilized by argon and water vortex in a plasma chemical reactor. The water-argon DC-plasma torch offers the advantage of low plasma mass flow rate, high enthalpy and temperature allowing achievement of an optimal conversion ratio with respect to syngas production compared to other types of plasma torches [1].

Numerical model was created in the ANSYS FLUENT 2022 R1 software package [2]. The model is fully three-dimensional, stationary, with Euler-Lagrange formulation for the gas and solid phases. The flow is subsonic, compressible and the plasma regions are considered to be in LTE. The chemical scenario of gasification production is defined by two chemical reactions.

Results of gasification and syngas production from crushed wood show that gasification efficiency and syngas production decrease slightly with increasing particle diameter, while thermal inhomogeneity in the reactor volume is strongest for the largest particle diameter and decreases with decreasing wood particle size. High syngas content (~90%) was achieved for all studied currents (400-600 A) and wood particle diameters (0.2 mm - 20 mm), look at Fig. 1 as an example.

![Fig. 1. Mean mole fractions of CO for 0.2 mm (left) and 1 mm (right) wood particle diameters in a chamber middle-cross-section at 400 A.](image)

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**References**


The polymeric fractions included in electrical and electronic equipment (EEE) have advantages, such as reducing the weight of the devices and increasing their durability. Additives and fillings enhance the plastic properties. Among the additives are plasticizers, flame retardants, heat stabilizers, organic or inorganic pigments, and fillers. In a recent study, around 10,000 substances have been identified, with 2400 considered as substances of potential concern [1]. In the case of waste of EEE (WEEE), some substances have been restricted by the European Directive 2011/65/EU [2]. Currently, the Directive includes four elemental pollutants (Cd, Hg, Pb, and hexavalent Cr) and two substance families: polybrominated biphenyls (PBBs) and polybrominated diphenyl ethers (PBDEs). The last substances are chemical compounds added to plastics to delay the spread of fire in case of ignition [3]. The components that have been thought to be at risk for ignition are the polymeric parts close to the source of electricity. Therefore, flame retardants (FRs) became important among the producers of the polymeric materials for EEE [4, 5]. Mechanical recycling has been used for plastics, promoting their circular economy or closing the loop of this waste stream. The recyclates are products from plastic recycling, and they are used as polymeric raw material. The concern is that PBDEs have been found in toys and kitchen utensils produced from recyclates (black plastics) [6-8]. A segregation protocol could generate a stream of plastics (free of pollutants) available for high-value recycling [9]. The plastics containing toxic compounds could be sent to a destructive technology, such as plasma chemical technology.

References
Energy Balance of Thermal Plasma Processing of Materials

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Thermal plasma is an effective tool for material processing or waste decomposition. [1] It can be generated by many ways. A typical and common example is the generation by direct current electric arc. One of the recent methods is plasma generation by microwaves. Both methods are tested for many purposes at the Institute of Plasma Physics of the Czech Academy of Sciences in Prague in a semi-operational experimental plasma reactors where thermochemical reactions take place at very high temperatures (in the order of thousands of °C). Research activities focus on the gasification and pyrolysis of various types of organic and inorganic materials and wastes to produce secondary raw materials such as functional carbon black, carbon or iron in the form of nanoparticles, or synthesis gas (syngas) rich in hydrogen and carbon monoxide. Syngas can be a source of energy, hydrogen and other fuels or chemical compounds (hydrocarbons). The remaining secondary solid phase materials have the potential for a wide range of scientific and industrial applications, e.g. in civil engineering [2], pharmaceuticals and medicine (activated carbon), electronics (supercapacitors, electrodes), etc. In addition, nanoparticles are attractive for nanotechnology and the synthesis of new alternative materials that can be used in optics or energy-saving technologies. During our experimental campaigns, the energy balance is studied in detail with the aim of the optimising the process and minimising the energy losses. The previous energy balance approach only numerically evaluated the inputs and outputs of the system. However, a more detailed study of the energy balance inside the plasma jet interacting with a material can be helpful for better understanding the specific processes taking place inside the reactor during the process. Useful tools for this can be for instance the optical emission spectroscopy, particle velocity recording or the knowledge of material properties and chemical reactions. Examples of different plasma sources and input materials will be presented. Nevertheless, at the laboratory scale, the energy consumption is significant. [3] In the future commercial applications this bottleneck may be potentially overcome by using supply of excess energy mainly available for example from nuclear and renewable energy sources.

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References
Deep Cleaning of Syngas

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This work focuses on the deep cleaning of syngas, with a primary emphasis on the analysis of selected secondary fuels. The studied fuels include RDF (refuse-derived fuel), medical waste, sewage sludge, waste plastics and tires [1], [2], [3], [4]. Using the proposed computational model, it is possible to determine the theoretical composition of the output products from plasma gasification of these fuels. The obtained data is then used for the design of cleaning lines to remove unwanted impurities. Selected fuels, such as natural gas, biogas, and biomethane, are considered for the production of carbon composites and pure hydrogen from syngas through plasma pyrolysis. Furthermore, the work examines syngas cleaning technologies aimed at obtaining pure hydrogen.

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References

Contribution in Czech: Napájecí Zdroje pro Plazmatrony – Klasifikace a Princip (Power Supplies for the Plasma Torches – Classification and Basic Principles)

Antonín Musil, Václav Březina, Dominik Kralík, Petr Brom

This contribution aims to introduce plasma torches power supply equipment. Detailed discussions of the following points will be delivered:

1) The power supplies available. The age and related principle of their operation explained using diagrams.
2) Localization of the power supplies and their accessories (chokes, switching terminals etc.) in the building and their connection to various laboratories.
3) Evaluation of the individual sources in terms of interference to the electrical network and options for dealing with the situation.
A Two-layer Closable PDMS Microfluidic Device for Plant Roots Growth Observation

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The molecular biology of plant roots growth is interesting but very challenging from the point of experimentation. The simultaneous observation of the root growth and a protein expression thanks to protein fluorescence requires developing special engineering tools. Real-time observation of a plant root growth can be realized by placing a root of a model plant, for example, Arabidopsis thaliana, into a small microfluidic channel with a cross-sectional area matching the root dimension itself (e.g., the cross-section area is 500x110 micrometres for Arabidopsis). The microfluidic channel is then filled with nutrients. The root observation is performed directly using a camera mounted on the optical microscope. For that reason, the microfluidic device has to be transparent. Here, we use soft-lithography techniques based on polydimethylsiloxane (PDMS) to fulfil this requirement. In our case, we study the impact of different nutrients on the velocity rate of plant root growth. The developed microfluidic device thus contains pressure-actuated valves enabling to switch between different nutrients quickly. This feature allows us to study a real-time nutrient impact on plant growth and prevent unwanted diffusion between both nutrients.

In this contribution, we present the development of a multilayer closable PDMS microfluidic device that allows us to switch between two different nutrients. The PDMS device has two layers, a flow layer and a control layer. A flow layer contains the main flow channel with a cross-section area of 250x30 micrometres, inputs for nutrients and two main channels for root growth observation. The “root” channels have cross-section area of 1000x110 micrometres and length of 20 mm. A second layer called a control layer controls the flow direction in the main channel. The control layer is about 50 μm thick and is placed directly below the flow layer. It consists of seven channels that are filled and pressurized with mineral oil. The pressurized channel expands and closes the main channel underneath. By choosing which channel to pressurize, we can direct the flow in any branch of the microfluidic network. Both layers are made by PDMS casting against a master made of either SU-8 3035 or AZ IPS 6090 photoresists. The control and flow layers are bonded and fixed onto a microscopic cover glass using corona treatment.