Università di Roma "Tor Vergata"
Dipartimento di Scienze e Tecnologie Chimiche
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Ph. D Program in Materials for Sustainable Development
(Former denomination Materials for Health, Environment and Energy)

Ph D Students Yearly Report a.y.2023/2024
Abstracts

Cycle 39th

Student: Caka Ada
Thesis Tentative Title: The impact of the orthodontic treatment on the endodontically treated teeth with periapical lesions.

Abstract

It is very frequent the need of moving endodontically treated teeth and this movement is due to the periodontal ligament. Cementoblasts have no receptors for bone turnover mediators, but the osteoblasts located 0.25mm from the tooth have them. Orthodontic forces, very differently from the forces of occlusion and dental trauma, are characteristically very light, dissipating and applied slowly to the tissues. The application of an orthodontic force:
1. Compresses the cells, deforming its cytoskeleton, promoting a mechanical stress.
2. And at the same time, reduces the lumens of blood vessels with hypoxia in the area establishing a metabolic stress.
The stressed cells of the periodontal ligament release many mediators that alternately stimulate the resorption and the bone position on the ligament surface of the alveolar process, promoting local bone remodeling, fixating the tooth in a new position. The root resorption induced during orthodontic treatment will only occur if the applied forces also cause the death of cementoblasts with subsequent exposition of the root surface. The death of cementoblasts is necessarily associated to more intense forces that compress the vessels in certain areas of the periodontal ligament. The pulp tissues, on the other hand, do not suffer morphological and functional alterations during orthodontic movement,1,3 regardless of the type and intensity of the applied force. Thus, in the same way, if the canal is filled by endodontic material, it will also not cause any modification on the periodontal tissues before orthodontic movement. In cases of orthodontic movement of endodontically treated teeth in which a failure over months or years was detected, this fact must not be assigned to the performed tooth movement. The applied forces do not interfere on the pathogenicity and on the virulence of the associated microbiota, as well as on the biology of microbial biofilms and chronic inflammatory periapical lesions. The failure in these cases must be justified by the limitations inherent to the endodontic treatment and not by the fact that the tooth was subjected to orthodontic movement.
In other words, if a tooth properly endodontically treated is orthodontically moved and presents less or more root resorptions, this response is not directly related to the present orthodontic treatment.
In practically all situations, endodontically treated teeth to be orthodontically moved must be subjected to a careful evaluation about the adequate conditions or not of the endodontic treatment by the endodontist. In cases in which these conditions are considered inadequate or inappropriate an endodontic retreatment must be performed.
In teeth with chronic periapical lesions the frequency of irregular areas due to apical resorptions associated to it, is very high, increasing the possibility of persistence of microbial biofilms. The occurrence of failures on the hermetic closure of the apical opening due to natural anatomical irregularities can also justify these failures, as well as the presence of apical deltas, the used material and many other factors that affect the results. The possibility of failure in endodontically treated teeth with chronic periapical lesion is greater than in other situations. Seeing this situation coming, the aim of our study is: to verify the failure of a treatment in endodontically treated tooth is due to the orthodontic movement or due to an unproperly endodontic treatment.

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Student: Cammarota Ilaria
Thesis Tentative Title: Accuracy Of Dynamic Navigation for Implant Placement in Aesthetic Zone: A Prospective Clinical Trial

Abstract

The aim of the present study is to assess dynamic navigation guided surgery accuracy for implant placement in anterior zone. Patients requiring at least one implant in frontal area were treated between December 2020 and February 2024. Implant placement accuracy is evaluated superimposing pre-operative and post-operative Cone Beam Computed Tomographs and recording linear deviations at implant apex and platform and angular deviation. T-tests is performed to investigate implant site characteristic (Healed vs post-extractive) and type of arch (Maxilla vs Mandible) on the accuracy. P-value < 0.05 was the threshold for statistical significance.

Student: Cornale Michela
Thesis Tentative Title: Synthesis and characterization of La0.4Ca0.4Ti0.95Ni0.05O3 as fuel electrode for solid oxide cells (SOCs)

Abstract

This study shows the synthesis and characterization of La0.4Ca0.4TiO3 (LCT) an A-site deficient titanate oxide, and B-site doped La0.4Ca0.4Ti0.95Ni0.05O3 (LCTN). Different synthetic routes are presented. Structural and textural properties of the oxides are investigated by XRD. The structural stability after reduction in H2 is also assessed. The morphology is investigated by FE-SEM and Ni exsolution is revealed for LCTN sample. The electrical conductivity is measured in operating conditions (high T, reducing atmosphere). The electrochemical properties are evaluated on YSZ-based symmetric cells.

Student: Cuboni Valerio
Thesis Tentative Title: Materials in circular economy: from algae biomass waste to additive for bioplastics.

Abstract

The increase in plastic pollution is becoming an important concern for both the environment and human health. Today, the most promising alternative to fossil plastics is the development of thermoplastic materials from renewable polymers, called bioplastics. In this year, I have worked in the spinoff Splastica, to test the industrial extrusion properties of SP Milk, a protein-based bioplastics. Moreover, within a PRIN project, I investigated the positive effects of microalgae as a natural filler and dye for bioplastics, showing the benefit of microalgae to the mechanical properties of an existing material.

Student: Freni Claudia
Thesis Tentative Title: Molecular Simulations for Rational Aptamer Design: Advancing Biosensor Development through Optimized Aptamer Engineering

Abstract

Nucleic acid sequences exhibit exceptional versatility, being capable of forming diverse complex structures that are proven to be fundamental in bioanalytical applications. Split aptamers, composed of two or more short nucleic acid fragments, have emerged as a particularly promising tool in the development of advanced biosensors. This innovative approach involves strategically splitting an aptamer into independent fragments that reassemble upon recognizing a specific target molecule. The current project aims to predict and elucidate the underlying mechanisms of this splitting process through Molecular Dynamics simulations, followed by rigorous experimental validation.

Student: Freschi Lorenzo
Thesis Tentative Title: Study and development of innovative materials, new proton-conduction cell structures and geometries through alternative production techniques.

Abstract

Within the national project POR-H2, funded by the European Union-NextGenerationEU as part of the PNRR programme from the Italian Ministry of Environment and Energy Security, my PhD project started with the setup of a new laboratory for the manufacture of proton-conducting solid oxide fuel cells with conventional and PVD techniques. The first year's work focused on the laboratory organization and the synthesis of BaCe1-x-yZrxMyO3-δ perovskites (M = Y, Gd, Sm). Powders were characterized by XRD, TGA and SEM. Pellets were sintered in air varying temperature and dwell time to reach densification.

Student: Gosti Christian
Thesis Tentative Title: Development of potentiometric sensors for target analytes in water samples

Abstract

Calcium quantification represents a significant parameter to monitor the hardness of water samples. In this regard, potentiometric sensors based on Ion-Selective membrane, namely Ion-selective electrodes (ISEs), provide highly sensitive and selective for calcium ions detection given by electrochemical potential changes, related to its activity. Considering the cost-effectiveness and the reliability, potentiometric sensors offer a valid method for calcium monitoring in environmental applications.

Student: Marino Gabriel
Thesis Tentative Title: Development and Characterization of Structured Catalysts to Enhance Ammonia Synthesis for Chemical Energy Storage and Transportation.

Abstract

This project aims to develop structured catalysts with high mass and heat transport properties to enhance efficiency, flexibility, and productivity in alternative chemical energy processes. La- and Y-doped Ru/CeO_2 catalysts will be designed for ammonia synthesis at low temperatures (300-450°C), characterized by strong metal-support interactions and oxygen vacancies. The best-performing catalysts will be deposited on highly porous aluminum and silicon carbide foams or triply periodic minimal surfaces, improving mass and heat transfer.

Student: Montesani Lorenzo
Thesis Tentative Title: The Application of Biomaterials in Bone Regeneration

Abstract

Autologous tissue transplantation is currently considered the standard for hard and soft tissue regeneration due to its biocompatibility and ability to integrate without causing immune reactions. However, the limited availability of autologous tissue and the need for additional surgeries pose risks and inconveniences for patients. It is therefore essential to develop and use biomaterials that promote tissue regeneration in the dental field and that can be used before or during implant-prosthetic treatment.

Student: Pagano Giorgio
Thesis Tentative Title: Lanthanum nickelates as electrocatalysts for the oxygen evolution reaction

Abstract

Lanthanum nickelates (LaNiO3) are platinum group metal-free electrocatalysts with excellent electrocatalytic activity towards the oxygen evolution reaction (OER). In this work, LaNiO3 has been synthesized via coprecipitation and solution combustion synthesis with different bases and fuels, to evaluate the influence of the synthetic route on the electrocatalytic performance. Experimental results show that preparation method has a strong effect on OER activity, with solution combustion synthesis yielding the best results when a combination of glycine and citric acid is used.

Student: Paolo Prata
Thesis Tentative Title: Clinical and radiographical evaluation of two agenesis alveolar ridges of upper lateral incisors. A case report with 5 years follow up

Abstract

Besides the functional issues, lateral incisor agenesis represents a significant aesthetic drawback (1).
The decision about the treatment plan is complex due to the long-term success, which is not easy to achieve. It has to be discussed with the orthodontists to choose the closure, using permanent canines to replace the missing teeth, or maintaining the spaces, for example, with Maryland bridges or implants.
The main advantage of orthodontic gap closure is that this approach preserves the natural architecture of the complex and soft tissues. However, canines and premolar sizes and shapes should be adjusted to mimic the replaced teeth, eventually resorting to odontoplasty or veneers (13).
This article aims to show clinical protocols and procedures for the Split Crest without any graft.
The biggest problem in agenesis cases is the thickness of the bone, which is bucco-palatal and associated with the need for proper functional and esthetic rehabilitation.
In the case that we reported, because of the lack of thickness, we performed a minimally invasive split crest, which allowed us to correct the implant insertion with immediate loading by a temporary crown, just for aesthetic reasons.

Student: Spinelli Elodia
Thesis Tentative Title: Advanced nanostructured materials for the protection of artworks

Abstract

In the present research activity, Mesoporous Silica Nanoparticles (MSNs), Halloysite Nanotubes (HNTs) and Zein Nanoparticles have been selected and characterized as nanocarriers for the encapsulation of Thymol and Thyme Oil, high volatile species. The future intent is to disperse the loaded particles in protective materials for Cultural Heritage in order to protect the active compound from UV damage and tailor their kinetic release in air by sublimation and in water by leaching. The strategy is to design capping systems around the nanoparticles. For this reason, a cover around the MSNs was formed by the assembly of Tannic Acid and Fe^{III} coordination complex.

Student: Testarelli Luca
Thesis Tentative Title: Clinical, radiographical and biochemical evaluation of two different types of implant screw retained single crowns

Abstract

The objective of this study is to verify whether, 12 months after delivery, a significant difference in tissue response can be defined between these two different types of implant-retained single crown. During the time of clinical observation, at t0 (3 weeks from the delivery) , t3 (15 weeks after the delivery) and t6 (27 weeks from the delivery), both types of crowns performed satisfactorily from a clinical point of view. No statistically significant differences emerged. It is clearly possible to state that in light of the short observation period, it is not possible to state with certainty that there is no difference in terms of tissue inflammation of these two different types of screw-retained implant single-crown.

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Student: Tucci Fabio Giovanni

Thesis Tentative Title: Evaluating the Impact of Force Field Refinements on RNA Molecular Dynamics Simulations.

Abstract

This study evaluates the impact of CMAP corrections on the conformational dynamics of an RNA aptamerprotein complex using MD simulations with the OL3 force field. RMSD, RMSF, and PCA analyses focused on the C2' carbon atom show no significant differences between OL3 and OL3+CMAP simulations. The results suggest that CMAP corrections do not substantially alter the aptamer's global motions. Future work should explore additional structural properties and extend the analysis to more flexible RNA systems to fully assess the role of CMAP and verify the effect of the novel Stafix corrections on the RNA dynamics.

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