

Jornadas CeFEMA 2019

Report of Contributions

Contribution ID: 1

Type: **not specified**

Lattice QCD computations at CeFEMA

Monday 16 September 2019 14:00 (15 minutes)

The lattice QCD group at CeFEMA, researches hadronic physics with high performance computing. Lattice QCD starts from the QCD Lagrangian, and utilizes discrete techniques inspired in condensed matter physics. We develop CUDA codes to run in our servers with some of the NVIDIA graphics boards with the largest number of cores and memory. We generate our gluon configurations using Monte Carlo techniques, and collaborate with other groups to utilize configurations with quarks. To study colour confinement, a main open problem in theoretical physics, we have been specializing in the study of flux tubes, similar to the vortices of type II superconductors. Moreover have been studying exotic hadrons, such as tetraquarks and hybrids, for many years just a tantalizing prediction, and finally a confirmed experimental observation.

Presenter: BICUDO, Pedro (IST Lisboa)

Session Classification: Hadronics & QCD

Contribution ID: 2

Type: **not specified**

Quantum excitations of flux tubes

Monday 16 September 2019 14:15 (15 minutes)

This talk gives an overview about flux tubes on Lattice QCD. We will show the results for flux tubes at zero and finite temperature. Finally, we will present recent results of the excited spectrum of the gluonic fields produced by a static quark-antiquark pair.

Presenter: CARDOSO, Nuno (IST)

Session Classification: Hadronics & QCD

Contribution ID: 3

Type: **not specified**

Wilson Loop calculations

Monday 16 September 2019 14:30 (15 minutes)

I will talk about the calculation of Wilson's loop and how to extract the form on potential between quark and anti-quark without using smearing and compare the speed of the code on CPU and GPU. I will finish with a roughly talk on calculation of hybrids' properties which is the next phase of my work.

Presenter: SHARIFIAN, Alireza

Session Classification: Hadronics & QCD

Contribution ID: 4

Type: **not specified**

Interacting Quantum Matter, Non-Equilibrium and Topology

Monday 16 September 2019 11:00 (15 minutes)

This talk gives an overview of some of the recent work developed at CeFEMA in the area of Condensed Matter Theory.

My goal is to provide an integrated view of the different lines of research and their main motivation, as well as, to present the people working on them and the results they obtained. Finally, I would like to tell you about some of the future directions of our research.

Presenter: Prof. RIBEIRO, Pedro (CeFEMA/IST)

Session Classification: Condensed Matter Theory

Contribution ID: 5

Type: **not specified**

Quantum Open Systems with Matrix Product States

Monday 16 September 2019 11:15 (15 minutes)

The density matrix renormalization group is one of the most accurate numerical methods applied to the study of 1D quantum many body system. It can be framed as a variational problem by using what is called matrix product states (MPS). Its success is due to the fact that these variational representations exactly target area-law states, which in 1D require but a small number of parameters to be accurately described.

In this work we talk about the usefulness of using MPS to study quantum open systems, in particular to obtain steady states and compute the relevant physical observables that characterize them. We will also talk about future plans for using variational states to describe open systems with metallic contacts, a problem which eludes the more traditional approaches.

Presenter: OLIVEIRA, Miguel

Session Classification: Condensed Matter Theory

Contribution ID: 6

Type: **not specified**

Disordered topological systems

Monday 16 September 2019 11:30 (15 minutes)

We will discuss topological systems under the influence of disorder effects. We start by briefly introducing the topics of topological and disordered systems. We will then characterize the interplay between topology and disorder (quenched and annealed), providing examples of three different models characterized by the author: the disordered Haldane model, the Haldane-Falicov-Kimball model and a model of a nodal-line Weyl semimetal. All have in common that disorder effects are responsible for the existence of interesting non-trivial phases of matter in non-clean systems. Among these, are disorder and temperature-driven topological phases in the Haldane-like models, and a novel multifractal semimetallic phase in the nodal-line semimetal.

Presenter: GONÇALVES, Miguel

Session Classification: Condensed Matter Theory

Contribution ID: 7

Type: **not specified**

The vortex, the impurity, and the finitude of bound states

Monday 16 September 2019 11:45 (15 minutes)

We consider the problem of finding the bound-state spectrum of an impurity immersed in a weakly interacting two-dimensional Bose-Einstein condensate supporting a single vortex. We obtain approximate expressions for the energy levels and show that, due to the finite size of the condensate, the impurity can access only a finite number of physical bound states. By virtue of the topological quantisation of the vorticity and of the emergence of the Tkachenko lattice, this system is promising as a robust and scalable platform for the realisation of qubits. Moreover, it provides a potentially new paradigm for polaron physics in Bose-Einstein condensates and a glimpse towards the study of quantum turbulence in low-dimensionality systems.

Presenter: BRÁZ, João

Session Classification: Condensed Matter Theory

Contribution ID: 8

Type: **not specified**

Tracking Topological Phase Transitions

Monday 16 September 2019 12:00 (15 minutes)

We study the behavior of the fidelity and the Uhlmann connection in one and two- dimensional systems of free fermions with short range [1] as well as long range [2] amplitudes that exhibit non-trivial topological behavior. In particular, we use the fidelity and a quantity closely related to the Uhlmann factor in order to detect phase transitions at zero and finite temperature for topological insulators and superconductors. We show that at zero temperature both quantities predict quantum phase transitions: a sudden drop of fidelity indicates an abrupt change of the spectrum of the state, while the behavior of the Uhlmann connection signals equally rapid change in its eigenbasis. At finite temperature, the topological features are gradually smeared out, indicating the absence of finite-temperature phase transitions, which we further confirm by performing a detailed analysis of the edge states. Moreover, we performed both analytical and numerical analysis of the fidelity susceptibility in the thermodynamic limit, providing an explicit quantitative criterion for the existence of phase transitions.

Presenter: AMIN, Syed Tahir**Session Classification:** Condensed Matter Theory

Contribution ID: 9

Type: **not specified**

NMR Relaxometry in Complex Soft-Matter Systems: Experimental Results and Model Fitting

Tuesday 17 September 2019 11:10 (10 minutes)

Molecular order and dynamics of the CB-C9-CB liquid crystalline dimer exhibiting the nematic (N) and the twist bend nematic (Ntb) phases [1-2] were investigated by proton NMR spectroscopy, using fields of 0.78 T and 7.04 T, and relaxometry. The first relaxometry experiments for a very wide Larmor frequency domain (8 kHz–300 MHz) on this system, using a combination of standard and fast field cycling NMR techniques, were performed. The spectroscopy results in the Ntb phase allowed us to probe the local molecular orientation relative to the Ntb helix axis. The relaxation data were analyzed considering order director fluctuations (ODF), molecular self-diffusion (SD) and local molecular rotations/reorientations (R) relaxation mechanisms. Global fits of theoretical relaxation models, as a function of temperature and Larmor frequency, for the phases under investigation, allowed for the determination of rotational correlation times [3], diffusion coefficients, viscoelastic parameters, correlation lengths and activation energies (in the case of thermally activated mechanisms) [4]. A clear difference between the structures of the N and Ntb phases was detected from the results of proton spin–lattice relaxation through distinct temperature and frequency dependencies' signatures of the collective modes. Significant pre-transitional effects were observed at the N–Ntb phase transition both from relaxometry and spectroscopy data. The experimental results correlate to data and models for comparable liquid crystalline systems.

[1] V. Borshch, Y. K. Kim, J. Xiang, M. Gao, A. Jakli, V. P. Panov, J. K. Vij, C. T. Imrie, M. G. Tamba, G. H. Mehl and O. D. Lavrentovich, *Nat. Commun.*, 2013, 4, 2635.

[2] I. Dozov, *Europhys. Lett.*, 2001, 56, 247–253.

[3] A. Ferraz, J. Zhang, P. J. Sebastião, A. C. Ribeiro and R. Y. Dong, *Magn. Reson. Chem.*, 2014, 52, 546–555.

[4] P.J. Sebastião, C. Cruz, A.C. Ribeiro, “Advances in Proton NMR Relaxometry in Thermotropic Liquid Crystals” in *Nuclear Magnetic Resonance Spectroscopy of Liquid Crystals*, pp. 129-167, Ed. R. Dong, World Scientific Co., ISBN: 978-981-4273-66-4, 2009

Presenter: SEBASTIÃO, Pedro

Session Classification: Complex Fluids NMR

Contribution ID: 10

Type: **not specified**

1H NMR relaxation study of molecular dynamics in the nematic and NT-B phases formed by the liquid crystal dimer DTC5C7

Tuesday 17 September 2019 11:20 (15 minutes)

Liquid crystalline dimers linked by an odd numbered hydrocarbon spacer are of significant interest due to their LC polymorphism, specifically due to the formation of the Ntb phase [1] in some of the LC dimers. The Ntb phase has been discovered recently and, the detailed description and understanding at the molecular level in this phase is still qualitative. In this work, by using a range of NMR techniques, we have addressed this question.

Here, we present the results of a detailed proton NMR relaxation study of molecular dynamics using the conventional and fast field cycling NMR techniques over a wide range of Larmor frequencies [2] in the dimer DTC5C7 [3]. This material and related difluoroterphenyl (DTC5Cn) compounds have already been investigated by a range of techniques including the X-ray diffraction techniques, modulated and conventional DSC, a range of electro-optical methods, and NMR spectroscopy [3-6]. With this investigation, we expand the current knowledge on these systems as the proton NMR relaxation techniques provide a detailed insight of physical properties such as correlation times, viscoelastic parameters and correlation lengths related to the structural properties of the studied mesophases.

Acknowledgements:

Portuguese Science and Technology Foundation (FCT) through CeFEMA strategic project UID/CTM/04540/2018. European Union and FCT through Grant M-ERA-NET2/0006/2016 (CellColor) and the EPSRC (project EP/M015726/1).

[1] V. P. Panov et al., Phys. Rev. Lett., 105, 167801 (2010); C. S. P. Tripathi et al., Phys. Rev. E, 84, 041707 (2011); M. Cestari et al., Phys. Rev. E, 84, 031704 (2011).

[2] A. Aluculesei et al., Phys. Chem. Chem. Phys., 21, 4523 (2019).

[3] S. M. Salili et al., Phys. Rev. Lett., 116, 217801 (2016);

[4] J. W. Emsley et al., Phys. Chem. Chem. Phys., 18, 9419 (2016);

[5] W. D. Stevenson et al., Phys. Chem. Chem. Phys., 19, 13449 (2017);

[6] W. D. Stevenson et al., Phys. Chem. Chem. Phys., 20, 25268 (2018).

Presenter: KUMAR, Anant

Session Classification: Complex Fluids NMR

Contribution ID: 11

Type: **not specified**

NMR study of the molecular dynamics in magnetic and non-magnetic ionic liquids

Tuesday 17 September 2019 11:35 (15 minutes)

Recent studies [1-3] have shown a considerably large paramagnetic relaxation enhancement associated with mixtures comprising magnetic ionic liquids (MILs) (based on either [Aliquat]⁺ or [P66614]⁺ cations and on a [FeCl₄]⁻ anionic complex) and their analogous ionic liquids (respectively [Aliquat][Cl] and [P66614][Cl]). These properties were, however, destroyed when the same amount of phosphonium-based MIL was dissolved in dimethyl sulfoxide (DMSO), possibly because this solvent is not as structured as an ionic liquid and, therefore, does not allow for a coupling of the iron spins [2]. In order to gradually attenuate this effect, ternary mixtures of IL, MIL (also at 1% (v/v) concentration) and DMSO-d₆ were studied and it became clear that, for smaller DMSO concentration (up to 10% (v/v)) as well as for temperatures ranging from 5 to 70°C, the effect on the paramagnetic relaxation is almost negligible [3]. Furthermore, all these studies show a clear dependence of the diffusion coefficient (and, hence, of the viscosity) on the applied magnetic field. Additionally, the effect of a different metal containing anionic complex (GdCl₃) was evaluated with the [P66614]⁺ at different temperatures. At ten times less concentration, the gadolinium-based MIL presents a comparable relaxation enhancement to that observed with iron and at lower magnetic fields. The effect at different temperatures (5-70 °C) was also analyzed as well as the behavior of the diffusion coefficient and the viscosity at different external magnetic fields.

[1] Carla Daniel et al., J. Phys. Chem. B, 2013, 117 (39), pp 11877–11884

[2] Carla Daniel et al., J. Phys. Chem. B, 2015, 119 (35), pp 11740–11747

[3] Maria Beira et al., J. Phys. Chem. B, 2017, 121 (51), pp 11472-11484

Presenter: BEIRA, Maria

Session Classification: Complex Fluids NMR

Contribution ID: 12

Type: **not specified**

Hemocompatible nanostructured membranes for artificial organs

Monday 16 September 2019 09:35 (25 minutes)

Artificial Organs are generally associated to clinically well-established membrane-based treatments that assure in extracorporeal blood circulation devices the separation functions of a failing organ like the hemodialyzer (HD) for the kidney or the membrane blood oxygenator (MBO) for the lungs.

Current available medical devices used in these treatments are implicated with severe long-term side effects associated to the fact that the membranes employed present poor hemocompatibility. One of the main research areas of the Laboratory of Membrane Synthesis and Processes is the development of new membranes with tailored optimal surface/bulk morphologies with high flow/mass transfer associated with the metabolic functions of the kidney and artificial lung and enhanced hemocompatibility capable of sustaining kidney and lung support for lengthier periods.

Presenter: Dr FARIA, Mónica

Session Classification: Health

Contribution ID: 13

Type: **not specified**

Tailoring asymmetric structures of cellulose acetate/silica membranes for the artificial kidney

Monday 16 September 2019 10:00 (15 minutes)

The cellulose acetate (CA) membranes, developed in the early 1960s by Loeb and Sourirajan [1] for sea water desalination, are prepared by the wet phase inversion method [2] which is responsible for creating an asymmetric structure. The structure is composed of a thin skin dense layer that determines the membrane selective characteristics and a porous sublayer which provides mechanical support [3]. The wet phase inversion method allows the synthesis of asymmetric membranes, from a myriad of polymers, with a diverseness of structures accountable for a broad spectrum of separation characteristics. Hence, the specific selective permeation properties of a membrane can be tailored through the formulation of the casting solutions composition - in the polymer/solvent system - and control of the casting parameters - evaporation time and coagulation media [3]. This versatility allows the synthesis of hybrid membranes of CA and silica (SiO₂) [4], CA/SiO₂ membranes, by coupling the wet phase inversion [2] with the sol-gel [5] techniques. Their usage is envisaged in the purification of blood, by ultrafiltration (UF), for the artificial kidney. The present work addresses the synthesis of hybrid CA/SiO₂ membranes, which are either submitted to a solvent exchange [6] post-treatment or a surfactant mixtures conditioning [7]. The assessment of post-treatments on membrane structure modification is performed by the membranes characterisation in terms of (1) selective permeation characteristics: hydraulic permeability, rejection to salts, neutral macromolecules and molecular weight cut-off (MWCO); and (2) water order and dynamics within the membranes porous structure by 2H NMR spectroscopy, 1H NMR relaxometry and diffusometry [8]. In conclusion, the post-treatment by solvent exchange caused a shrinkage of the membranes porous structure leading to different permeation characteristics than those of untreated membranes. Additionally, the conditioning with surfactant mixtures presented minimal dissimilarities on the membrane's permeation properties.

References

- [1] S. Loeb and S. Sourirajan, "Sea Water Demineralization by Means of an Osmotic Membrane," *Advances in Chemistry*, vol. 38, pp. 117–132, jan 1963.
- [2] B. Kunst and S. Sourirajan, "An approach to the development of cellulose acetate ultrafiltration membranes," *Journal of Applied Polymer Science*, vol. 18, no. 11, pp. 3423–3434, 1974.
- [3] P. M. Bungay, H. K. Lonsdale, and M. N. de Pinho, eds., *Synthetic Membranes: Science, Engineering and Applications*. Dordrecht: Springer Netherlands, 1986.
- [4] G. Mendes, M. Faria, A. Carvalho, M. C. Gonçalves, and M. N. de Pinho, "Structure of water in hybrid cellulose acetate-silica ultrafiltration membranes and permeation properties," *Carbohydrate Polymers*, vol. 189, no. October 2017, pp. 342–351, 2018.
- [5] C. J. Brinker and G. W. Scherer, *Sol-Gel Science*. San Diego: Academic Press, 1990.
- [6] A. Lui, F. D. F. Talbot, A. Fouda, T. Matsuura, and S. Sourirajan, "Studies on the solvent exchange technique for making dry cellulose acetate membranes for the separation of gaseous mixtures," *Journal of Applied Poly-*

mer Science, vol. 36,

no. 8, pp. 1809–1820, 1988.

[7] K. D. Vos and F. O. Burris, “Drying cellulose acetate reverse osmosis membranes,” *Industrial and Engineering Chemistry*

Product Research and Development, vol. 8, no. 1, pp. 84–89, 1969.

[8] M. J. Beira, M. P. Silva, M. Condesso, P. Cosme, P. L. Almeida, M. C. Corvo, P. J. Sebastião, J. L. Figueirinhas, and

M. N. de Pinho, “Molecular order and dynamics of water in hybrid cellulose acetate–silica asymmetric membranes,”

Molecular Physics, vol. 117, no. 7-8, pp. 975–982, 2019.

Presenter: PEREIRA DA SILVA , Miguel

Session Classification: Health

Contribution ID: 14

Type: **not specified**

Modeling of macro-cryoconcentration phenomena during the freezing of bio-pharmaceutical aqueous solutions

Monday 16 September 2019 10:15 (15 minutes)

Modelling unstirred freezing of aqueous solutions with volumes between few millilitres and hundreds of litres is very useful in a multitude of applications. Aqueous solutions are frozen, for instance, in the food or biopharma industries to preserve the main ingredients. In these two applications, the quality of the frozen product depends on the adequate design of the freezing systems. To get realistic predictions, we need to take into account the different phenomena that take place when ice crystal forms. During the freezing process, ice crystals grow and entrap a concentrated solution, forming what is called a mushy layer. At the same time, this mushy layer expands and the mixture-air interface deforms. The concentrated solution inside the mushy layer tends to percolate as the mushy layer grows, disrupting the macro-homogeneity of the frozen product. The heat transfer modelling in this system needs also to take into account important differences in the heat capacity of the ice and of the liquid.

We describe in this presentation a VOF solver based on the OpenFOAM 5.0 library to model the freezing of binary aqueous solutions. The mixture-air and mushy layer-liquid solution interfaces are captured by using the VOF model approach, where the volumetric fraction of the liquid and of the ice varies continuously in space. The percolation of the concentrated binary solution is simulated using an equation similar to the Kozeny-Carman equation. The ice mass source was computed based on a local weight function that concentrates the ice mass source near the ice front. This new methodology contributes to enhance the numerical stability of the solver. The energy equation that was implemented takes into account the heat capacity of the liquid solution and of the ice. This model uses thermo-physical properties of the aqueous solution, which are easy to measure or to find in the literature. The percolation model, however, has a constant that must be found for each binary solution, based on the measurement of the distribution of solution concentration in frozen mixture.

The solver is validated with experimental data obtained during the freezing of 10% (w/w) dimethyl sulfoxide (DMSO), in a cylindrical container with cooled walls, in the range of 1 mL to 100 mL. The experimental Temperature time-profiles in the geometric centre of the cylinder are compared with the solver predictions.

VÍTOR GERALDES¹, FRANCISCO BARATA², MIGUEL RODRIGUES³, PEDRO REGO⁴

1,2) CeFEMA, Department of Chemical Engineering, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

3) CQE, Centro de Química Estrutural, Department of Chemical Engineering, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

4) Smartfreez Lda. Av. Jacques Delors, Ed. Inovação II, Incubadora Taguspark, 411, 2740-122 Porto Salvo Portugal

Presenter: BARATA, Francisco

Session Classification: Health

Contribution ID: 15

Type: **not specified**

LignoPower: technology for lignin isolation by black liquor electrolysis

Monday 16 September 2019 15:45 (15 minutes)

Black liquor is a secondary product of pulp mills that contains a considerable amount of organic compounds. Currently, this by-product is burned in recovery furnaces, in order to recover chemicals and to generate energy. However, during production peaks, the black liquor produced could exceed the capacity of those equipment, being a bottleneck in pulp production. Considering that, several processes have been studied, in order to give an economical attractive destiny to this black liquor excess. Lignin is an aromatic polymer, which is present in a considerable concentration in black liquor. It can be used as raw material for different applications, namely as a phenol substitute in phenolic resins, as a complementary crosslinker in epoxies, as an additive for biodegradable plastic and even as binding agent [1,2]. Taking this into account, different methods to recover the black liquor lignin have been studied in the last few years, namely acidification, membrane processing and electrolysis [2,3]. The electrolysis is a promising technology since it is a low-cost process and simple, since it does not involve the use of chemicals. During electrolysis it is observed the oxidation of the lignin at the anode side, while at the cathode side occurs the generation of hydrogen, a clean fuel whose combustion just produces water and energy [4]. Thus, in this work different low-cost electrode materials are tested as anodic electrodes for a black liquor electrolyser and their catalytic activity compared.

Acknowledgements

The authors would like to thank the Portuguese Foundation for Science and Technology (FCT) for PhD grant SFRH/BD/137470/2018 (R.C.P. Oliveira) and for contract no. IF/01084/2014/CP1214/CT0003 under IF2014 Programme (D.M.F. Santos). This work was carried out under the Project Impactus – Innovative products and technologies from eucalyptus, Project N.º 21874 funded by Portugal 2020 through European Regional Development Fund (ERDF) in the frame of COMPETE 2020 nº246/AXIS II/2017.

References

- [1] D. Stewart, Lignin as a base material for materials applications: Chemistry, application and economics, *Ind. Crops Prod.* 27 (2008) 202–207.
- [2] R.C.P. Oliveira, M. Mateus, D.M.F. Santos, Black liquor electrolysis for hydrogen and lignin extraction, *ECS Trans.* 72 (2016) 43–53.
- [3] R.C.P. Oliveira, M. Mateus, D.M.F. Santos, Chronoamperometric and chronopotentiometric investigation of Kraft black liquor, *Int. J. Hydrogen Energy* 43 (2018) 1–7.
- [4] C-J. Winter, Hydrogen energy – Abundant, efficient, clean: A debate over the energy-system-of-change, *Int. J. Hydrogen Energy* 34 (2009) S1-S52.

Presenter: OLIVEIRA, Raísa

Session Classification: Energy

Contribution ID: 16

Type: **not specified**

Zero-valent ruthenium nanoparticles incorporated in Fe-BTC metal-organic framework as anode catalyst for direct borohydride-peroxide fuel cell

Monday 16 September 2019 16:00 (15 minutes)

As the human exigency for energy is constantly increasing, the world is facing excessive use of fossil fuels as energy sources known to have undesirable impact on human lives and environment. Hence, with the development of modern society, the need for clean energy and shift to low carbon economy has also been growing. In order to deal with those issues, researchers have introduced different fuel cell designs as a promising class of sustainable power sources. Thus, direct borohydride fuel cells, DBFCs, have been receiving great attention of the science community [1]. Despite many advantages, practical application of those devices has been hampered due to their high investment cost, mainly related to high price of anodic catalyst used (usually, a precious metal). To overcome this issue, development of efficient, low cost and durable electrocatalysts is required. That can be achieved by alloying noble metals with other metals of lower price or by using a support with high surface area and capacity to stabilize metal particles [2].

Metal-organic frameworks (MOFs) have emerged as novel materials showing immense potential for energy conversion application due to their unique attributes such as ultrahigh porosity and internal surface area, good thermal stability and versatile framework, as well as their cheap and high-yield synthesis methods. Herein, Fe-BTC (Basolite F-300) MOF was synthesized and used as host material to stabilize guest ruthenium(0) nanoparticles (Ru@ Fe-BTC), which were fabricated by following previously reported synthesis protocol [3]. The present work aims at evaluating the performance of the prepared materials as electrocatalysts for borohydride oxidation reaction (BOR), since Ru alloyed with non-precious metals (e.g., Ni) or dispersed on high surface area carbon, has already been proven to have good electrocatalytic activity towards BOR [4, 5].

The electrocatalysts were characterized by using multi-pronged techniques, such as inductively coupled plasma optical emission spectrometry (ICP-OES), powder X-ray diffraction analysis (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and N₂-ads.-des. technique. Cyclic and linear scan voltammetry techniques were used to examine the catalytic activity of the materials for BOR at different temperatures (25 –65 °C) and concentrations (0.01 – 0.12 M NaBH₄). For all experiments 2 M NaOH was used as supporting electrolyte to guarantee the alkalinity of the media. BOR kinetic parameters, such as charge transfer coefficient, number of exchanged electrons, activation energy and order of reaction were calculated and compared with those reported in the literature. A small-scale DBFC (using hydrogen peroxide as a liquid oxidant) was assembled using the Ru nanoparticles immobilized on MOFs as an anodic catalyst and the fuel cell performance was assessed at different temperatures.

The authors would like to thank the Portuguese Foundation for Science and Technology (FCT) for the research grant within project UID/CTM/04540/2013 (G. Backović) and for contract IST-ID/156/2018 (B. Šljukić) and contract no. IF/01084/2014/CP1214/CT0003 under IF2014 Programme (D.M.F. Santos).

[1] D.M.F. Santos, C.A.C. Sequeira, *Renew. Sustain. Energy Rev.* 15 (2011) 3980-4001.

[2] R.C.P. Oliveira, J. Milikić, E. Daş, A.B. Yurtcan, D.M.F. Santos, B. Šljukić, *Appl. Catal. B, Environ.* 237 (2018) 1-12.

[3] G. Majano, O. Ingold, M. Yulikov, Gunnar Jeschke, Javier Pérez-Ramírez, *CrystEngComm* 15 (2013) 9885-9892.

[4] M.G. Hosseini, R. Mahmoodi, *New J. Chem.* 41 (2017-) 13408-13417.

[5] C. Grimmer, R. Zacharias, M. Grandi, B. Cermenek, A. Schenk, S. Weinberger, F.A. Mautner, B.

Bitschnau, V. Hacker, J. Phys. Chem. C 119 (2015) 23839-23844.

Presenter: BACKOVIC , Gordana

Session Classification: Energy

Contribution ID: 17

Type: **not specified**

Organic load removal from swine breeding wastewater using electrochemical oxidation

Monday 16 September 2019 16:15 (15 minutes)

Swine wastewater (SW) is a complex substrate that contains varying amounts of micronutrients (nitrogen and phosphorus compounds), as well as organic matter. The need for removing these pollutants from SW is undeniable to avoid their dangerous accumulation on the environment. Most farms use biological methods (e.g. anaerobic lagoons) as standard practice for wastewater treatment [1]; however, though very cost-effective, the treated wastewater may not always comply with environmental regulations due to significant efficiency losses when dealing with high strength effluents. Long retention times, chemical stability of refractory organic molecules, and the complexity of their degradation processes by biological pathways are other important limitations. Based on this, alternative oxidation methods have been tested to replace or complement biological treatment methods. Electrochemical methods such as electrooxidation (EO) have the advantage of being rapid, highly efficient, and more selective. When using EO, organic compounds are removed either by direct or indirect oxidation. In direct electron transfer, pollutants are adsorbed at the anode surface after diffusion from the bulk solution and then oxidized to other products [2]; in indirect electron transfer, which occurs in the potential region of oxygen evolution, pollutants are degraded either at the electrode surface by mediation of hydroxyl radicals and/or on the bulk solution by, for example, active chlorine [2]. These electrogenerated oxidants have considerably oxidative standard reduction potential and react rapidly with most electron-rich organic and nitrogen compounds causing their full conversion into CO₂ and inorganic ions [3]. The main disadvantage of this method is its high energy cost, but the interest in EO has greatly increased in recent years with several applications to wastewaters with high COD and low biodegradability [4,5]. Thus, this work aims to investigate the removal of organics from SW using electrooxidation. A statistical technique known as the Taguchi method is used to study the effects and optimize the operation parameters (i.e., initial pH, current density, and reaction time) that affect the process in terms of COD removal.

[1] T. F. Ducey and P. G. Hunt, "Microbial community analysis of swine wastewater anaerobic lagoons by next-generation DNA sequencing," *Anaerobe*, vol. 21, pp. 50–7, 2013.

[2] C. A. Martínez-Huitle, M. A. Rodrigo, I. Sirés, and O. Scialdone, "Single and Coupled Electrochemical Processes and Reactors for the Abatement of Organic Water Pollutants: A Critical Review," *Chem. Rev.*, vol. 115, no. 24, pp. 13362–13407, 2015.

[3] E. Isarain-Chávez et al., "Comparative electrochemical oxidation of methyl orange azo dye using Ti/Ir-Pb, Ti/Ir-Sn, Ti/Ru-Pb, Ti/Pt-Pd and Ti/RuO₂ anodes," *Electrochim. Acta*, vol. 244, pp. 199–208, 2017.

[4] M. Panizza and C. A. Martínez-Huitle, "Role of electrode materials for the anodic oxidation of a real landfill leachate –Comparison between Ti–Ru–Sn ternary oxide, PbO₂ and boron-doped diamond anode," *Chemosphere*, vol. 90, no. 4, pp. 1455–1460, Jan. 2013.

[5] A. Fernandes, E. Catalao, L. Ciriaco, M. J. Pacheco, and A. Lopes, "Electrochemical treatment of leachates from sanitary landfills," *J. Electrochem. Sci. Eng.*, vol. 3, no. 3, pp. 125–135, 2013.

Acknowledgements

G. Lourinho would like to thank the Portuguese Foundation for Science and Technology (FCT) regarding the grant SFRH/BDE/111878/2015.

Presenter: LOURINHO, Gonçalo

Session Classification: Energy

Contribution ID: 18

Type: **not specified**

The influence of glaze on the tribological properties of zirconia dental pieces obtained by subtractive and additive manufacturing

Tuesday 17 September 2019 09:35 (15 minutes)

Ceramic based prosthetic materials are highly used for the repairing/replacing of a damaged/missing tooth, due to their suitable mechanical and aesthetic properties, chemical stability and biocompatibility. Additive manufacturing (AM) has emerged as new methodology to obtain long term 3D dental pieces at low cost, decreasing the materials' waste and production time relatively to the conventional manufacturing methods. Generally, ceramic restorations are coated with a ceramic glaze paste, which is applied over the surface in order to improve its aesthetic properties.

The aim of this study is to evaluate the potential of additive manufacturing (AM) to produce reliable zirconia dental structures and the influence of glazing on the tribological performance of the obtained samples. To validate the possibility of using such technique, the results were compared with those obtained with samples produced by a conventional subtractive manufacturing (SM) method.

Zirconia samples produced by both methods were sintered at 1500°C, polished to obtain the same surface finishing and glazed. Density, porosity, Vickers hardness, toughness and roughness measurements were performed and chewing simulation tests against dental human cusps were carried out in artificial saliva, before and after glazing. The counter-faces' wear was quantified and the wear mechanisms investigated.

SM and AM samples present similar density and surface roughness. AM samples show a higher surface porosity, but lower hardness and toughness than SM. The glaze coating led to a significant decrease of surface hardness, to a value similar to enamel. After the chewing simulation tests, no wear was found for both unglazed SM and AM samples. However, the cusps suffered a significant volume reduction, which was higher for the SM samples. Concerning the glazed samples, the wear tests revealed that both the cusps and the glazed surfaces suffered wear. The cusps' wear was significantly higher in tests with the glazed samples. The dental and glaze main wear mechanisms were abrasion and delamination. Dental material adhesion to the zirconia samples was also observed both for glazed and unglazed samples.

In conclusion, AM is a promising technique to produce dental pieces, but material's porosity is still a concern, since it may affect the materials' toughness. The use of glaze led to similar results for SM and AM. However, it increases the material and cusps' wear.

A.C. Branco^{1*}, M. Polido², R.Colaço^{2,3}, C.G. Figueiredo-Pina^{2,3,4}, A.P. Serro^{1,2}

1 Centro de química estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal;

2 Centro de investigação Interdisciplinar Egas Moniz, Instituto Universitário Egas Moniz, Quinta da Granja, Monte de Caparica, 2829-511 Caparica, Portugal;

3 IDMEC e departamento de Engenharia Mecânica, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal;

4 Centro de Física e Engenharia de Materiais Avançados, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

Presenter: CATARINA BRANCO, Ana

Session Classification: Materials Processing

Contribution ID: 19

Type: **not specified**

Ageing of single crystalline laser deposited René N4 nickel superalloy

Tuesday 17 September 2019 10:05 (15 minutes)

The outstanding creep and thermal fatigue resistance of the high-temperature alloys used in the hot section of gas turbine engines for the aerospace and energy production industries are ensured by a single-crystalline structure and a microstructure composed of cuboidal γ' phase precipitates densely distributed in a γ phase matrix, which is generated during a complex ageing treatment. This microstructure must also be present in the overlay layers deposited when single-crystal Ni superalloy components are repaired by methods such as laser powder deposition. However, when conventional aging treatments are applied to laser deposited René N4, the precipitates formed do not present the desired cuboid shape. Detrimental Topological Closed Packed (TCP) compounds tend to form in the interdendritic regions of the deposited material microstructure as well.

The aim of the present work was to find an explanation for the formation of these undesired microstructural features and to devise an ageing process capable of achieving a suitable structure. Walls of laser deposited René N4 were built on René N5 single-crystal substrates. The crystallographic and metallographic structures of the deposited material were analysed in order to find the processing windows that optimise the properties of the deposited material. After obtaining single-crystal walls with the crystallographic orientation of the substrate, their microstructure was studied by SEM, SEM-EDS and SEM-EBSD in order to characterise the mosaicity of the crystal and the solute partition in the dendritic structures, detect TCP particles and identify their formation conditions.

Heat treatments capable of creating fine cuboidal γ/γ' microstructures in the deposited material and in the substrate were devised and tested. The best microstructures were obtained by a three-step thermal cycle where the ageing treatment is preceded by a homogenisation annealing, which eliminates the TCP particles and reduces the dendritic chemical segregation which originates the formation of precipitates with non-cuboidal shapes.

Presenter: CARDOSO, José

Session Classification: Materials Processing

Contribution ID: 20

Type: **not specified**

Influence of laser surface nanotexturing on the friction of silicon in dry sliding conditions

Tuesday 17 September 2019 10:20 (15 minutes)

The aim of the present work was to understand the role of Laser-Induced Periodic Surface Structures (LIPSS) on the friction behavior of silicon. A uniform LIPSS texture was generated on Si using femtosecond pulsed laser radiation. The wear tests were performed using a reciprocating ball-on-flat nanotribometer in dry sliding conditions and using polytetrafluoroethylene (PTFE) as counterbody. Wear tests were performed parallel and perpendicularly to the LIPSS orientation and compared to the polished Si case tested under the same conditions.

In the Si/PTFE tribosystem, wear is dominated by the plastic deformation of the PTFE counterbody. For the polished Si specimen, a discontinuous and 'lumpy' PTFE transfer layer forms on the Si surface, leading to relatively high values of the friction coefficient. Texturing leads to values of the friction coefficient similar to those of the polished Si for the parallel sliding direction, due to the abrasive action of the textured surfaces and discontinuous transfer film. When sliding perpendicularly to the LIPSS, a more uniform and adherent PTFE transfer film forms, leading to a friction coefficient that is independent of the applied load and lower than for the two previous cases.

Presenter: ALVES LOPES, Isabel

Session Classification: Materials Processing

Contribution ID: 21

Type: **not specified**

On the wear behaviour of LASER clad Colmonoy-6 coatings under corrosive media

Tuesday 17 September 2019 09:50 (15 minutes)

The process of laser cladding using Ni-Cr-B-Si-C alloy powders has gained relevance as a method to produce hardfacing coatings that provide excellent surface wear and corrosion resistance in a corrosive environment. However, under chemically aggressive media, the wear performance of such coatings is dependent on the synergic interaction between mechanical wear and electrochemical corrosion processes. In this work, a boron rich nickel alloy (Colmonoy-6) was deposited on a 316L stainless steel substrate through the process of laser cladding. Vickers microhardness measurements for both substrate and coating were realised using a 200g load. Polished coating and substrate samples underwent wear testing using sphere-on-plate reciprocation sliding conditions. The friction coefficient was measured continuously during all wear tests that were conducted under dry atmospheric conditions and under several aqueous corrosive media. XRD, SEM/BSE and EDS were used to characterise worn and unworn sample surfaces and wear losses were quantified through profilometry. Relatively to the substrate, results show that the coating presents adequate structure and improved wear behaviour for application under dry and severely corrosive environments. Light abrasion was identified as the main wear mechanism in NaOH and NaCl media. During wear in H₂SO₄ medium, the coating suffered a preferential phase dissolution and surface smearing of a ductile Ni phase. While all aqueous media reduced wear losses relatively to dry conditions, the best corrosion-wear resistance was measured for coatings tested in NaOH and NaCl media.

I. Rodrigues^{1,2}, B. Nunes^{2,3}, A. Almeida^{2,3}, R. Vilar^{2,3}, C. G. Figueiredo-Pina^{1,2}
¹CDP2T and Department of Mechanical Engineering, School of Technology of Setúbal, Instituto Politécnico de Setúbal, 2910-761 Setúbal, Portugal
²CeFEMA, Center of Physics and Engineering of Advanced Materials, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
³ Department of Chemical Engineering, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

Presenter: RODRIGUES, Ivan

Session Classification: Materials Processing

Contribution ID: 22

Type: **not specified**

Electrochemical Technologies for Tackling Energy and Environmental Problems

Monday 16 September 2019 15:35 (10 minutes)

Traditional technologies for dealing with domestic and industrial effluents are often expensive or lead to low treatment efficiencies. Electrochemical technologies offer several advantages over those methods and, for that reason, are receiving increasing importance. On the other hand, fossil fuel depletion and environmental concerns are putting electrochemical energy conversion and storage devices under the spotlights of both the scientific community and the general public.

Our research group in CeFEMA is developing different electrochemical technologies that handle problems both in the field of energy and the environment. This talk will briefly summarise the ongoing works, our network of collaborations, and our objectives for the upcoming years.

Presenter: SANTOS, Diogo (IST)

Session Classification: Energy