Center of Physics and Engineering of Advanced Materials

Newsletter December 2018

CeFEMA

Editorial

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João Figueirinhas

The CeFEMA newsletter highlights some of the recently developed research activities in materials science, condensed matter physics and strongly interacting systems, well illustrating the Center's quality and innovative character. This number focus the work of recently arrived CeFEMA members that bring to the Center their significant expertise in cutting edge rapidly growing areas, such as electrochemical energy conversion and storage, quantum simulation of strongly interacting systems or large-scale parallel computing techniques for hadronic and condensed mater physics.

Development of electrochemical energy storage/ conversion devices

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Electrochemical energy conversion plays an important role in the development of sustainable technologies to reduce use of fossil fuels and to minimize the global warming. Development of electrochemical energy storage/conversion devices goes into several directions: development of capacitors, development of batteries and development of fuel cells. Alkaline fuel cells are advantageous in many aspects, offering high operating potential as well as high efficiency, good energy density and wide temperature operating range. Among different factors affecting the chemical-electrical energy conversion, two are crucial: choice of anode material for the fuel oxidation and choice of cathode material for the oxygen reduction reaction (ORR). Ideally, oxygen reduction should proceed through a four-electron process as this yields water, in contrast to the two-electron process, which produces hydrogen peroxide, a reactive species that can attack the fuel cell components such as the membrane. However, typically large overpotentials are required for the direct reduction of oxygen at most electrode substrates which influences the overall performance of a fuel cell.

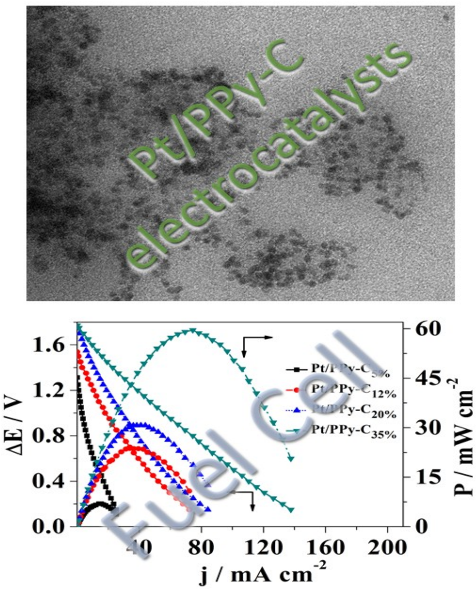

Fig. 1 - Evaluation of performance of fuel cells with different Pt/PPyC electrocatalysts."

Electrode modification for electrocatalysis of ORR is popular since electrode's activity can be significantly improved and the mentioned large ORR overpotential can be reduced through immobilization of an electrocatalyst onto electrode's surface. Many different materials have been proposed as electrocatalysts for oxygen reduction to water in fuel cells. Traditionally, such electrocatalysts are platinum – based, but their high cost limits large-scale application of fuel cells. Metal nanoparticles are normally supported on a high-surface area materials, such as carbon.

Materials Electrochemistry Group suggests use of metal oxides or conductive polymers as alternative supports, both pure or as composites with carbon. This line of research goes along with the CeFEMA aiming towards materials for sustainable energy applications reducing climate-changes impact of fossil fuels. Metal oxides are an obvious choice when considering electrode materials with high electrocatalytic activity for ORR and stability in highly alkaline solutions.

They have advantages of abundance, low cost, environmental friendliness and considerable electrocatalytic activity (though they could suffer from low surface area). As for conductive polymers, polyaniline, polythiophene, poly(3,4-ethylenedioxythiophene) and, particularly, polypyrrole are considered as the most promising for fuel cell applications due to their good electronic conductivity, as well as high chemical stability.

[1] R.C.P. Oliveira, J. Milikić, E. Daş, A.B. Yurtcan, D.M.F. Santos, B. Šljukić, Applied Catalysis B: Environmental 238 (2018) 454-464.
[2] M. Martins, J. Milikić, B. Šljukić, G.S.P. Soylu, A.B. Yurtcan, G. Bozkurt, D.M.F. Santos, Microporous and Mesoporous Materials 273 (2019) 286-293.

Quantum simulation of strongly interacting systems

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Hadronic Physics and Condensed Matter Physics have since several years experienced a cross-fertilization that has provided several powerful tools to treat hadrons and their interactions. Several few-body and many-body techniques have been used to study bound states and globally more extended systems as the ones created in high energy heavy ion collisions performed in accelerators on both sides of the Atlantic. In the latter case, several techniques developed in Condensed Matter Physics are presently used to study the QCD phase diagram and have led to several important discoveries such as the existence of superconducting phases in QCD, as well as more sophisticated phases related to non-trivial topological aspects of strongly interacting matter which can possibly be found in some stellar objects. Moreover, only the techniques developed for strongly correlated systems can allow for a reasonable treatment of QCD in systems with non-zero baryon chemical potential. The (newly-acquired) members of Cefema, João Seixas and Pedro Bicudo, have since many years worked in this area and are well-known internationally for their research in this domain.

But more recently the relation between Condensed Matter and Hadronic Physics has become even more tight in the realm of quantum simulation. It is well known that the particular characteristics of QCD make the simulation of strongly interacting systems particularly difficult to perform. In particular the simulation of such systems in cases where the baryonic potential is non-zero are essentially impossible to study using traditional Lattice Gauge Theory due to the well-known sign problem for the fermionic determinant. Recently [1] it has been shown that such problems could in principle be circumvented in quantum simulations. This has recently led a group of hadronic physicists in CeFema (J. Seixas, E. Ribeiro, Pedro Bicudo) to start a new line of research related to quantum simulation of hadronic systems. This new direction for the study of simple strongly interacting systems includes also Sofia Leitão and Yasser Omar from the IST and IT Quantum Technologies Group, Simone Montagero from the University of Padova (Italy) and Walter Vinci from the D-Wave company (Canada). Several companies have already shown strong interest in providing free computing time in their quantum processor to run our projects, which vouch for the quality of the work provided by our group. We believe this will be an important addition to the present lines of work in CeFema which will thus place the Center in the new frontiers in quantum computation and quantum simulation.

[1] Christine Muschik et al 2017 New J. Phys.19 103020

Hadronic and condensed mater physics studied with high performance computing

Pedro Bicudo

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Quantum Chromodynamics (QCD), the quantum field theory for quarks and gluons, fundamental sub-nuclear particles, has been the area of work for Pedro Bicudo. In CeFEMA, he works in new hadronic materials, the quantization of boson and fermion fields, symmetry breaking, and high performance computing with GPUs. In his PhD thesis, with his supervisor Emílio Ribeiro, he developed quark models with coupled channels and with spontaneous chiral symmetry breaking, to study for instance the mass generation of the visible universe. After exploring several hadronic phenomena with different colleagues, he then addressed the confinement problem with a new technique, lattice QCD. He then supervised the PhD thesis of Marco Cardoso and Nuno Cardoso, and with them he developed a lattice QCD group at IST. He also has been studying exotic hadrons with the Frankfurt University lattice QCD group of Marc Wagner. Theoretically, the main open problem of QCD is the confinement of quarks and gluons. This problem is reminiscent of superconductivity in condensed matter physics. However the gluons are charged, and they have a screening mass. Quarks and gluons cannot be observed in an isolated form, and they must be combined into hadrons, say mesons and baryons. Recently the evidence for tetraquarks in the experimental collaborations BELLE, BESIII and LHCb, after decades of searches, made exotic hadrons one of the most tantalizing subjects in physics. Exotic hadrons such as tetraquarks, pentaquarks, hybrids and glueballs constitute in a sense the new materials of hadronic physics. Because QCD cannot be solved with the usual perturbative techniques of particle physics, lattice QCD discretises the space-time of the universe with a lattice and utilizes techniques of statistical physics to simulate QCD phenomena. This approach combines mathematical beauty with the use of supercomputers. Since supercomputers can be extremely expensive to purchase and operate, our lattice QCD group at IST became expert in coding with the CUDA language, to run the codes in Graphic Processing Units (GPUs). Presently the most performant GPUs have thousands of processing cores and DDR6 ram memories, reaching tens of teraflops. They are most efficient in extremely parallel problems, typical of lattice QCD.

Fig. 2 illustrates two recent and promising studies. The tetraquark flux tubes, constitue a very beautiful evidence of confinement, are computed in Ref. [1] with pure gauge QCD, i.e. with no quark degrees of freedom. In Ref. [2], tetraquarks resonances are computed with static and dynamical quarks, exploring the poles of the scattering S matrix in the Riemann space.

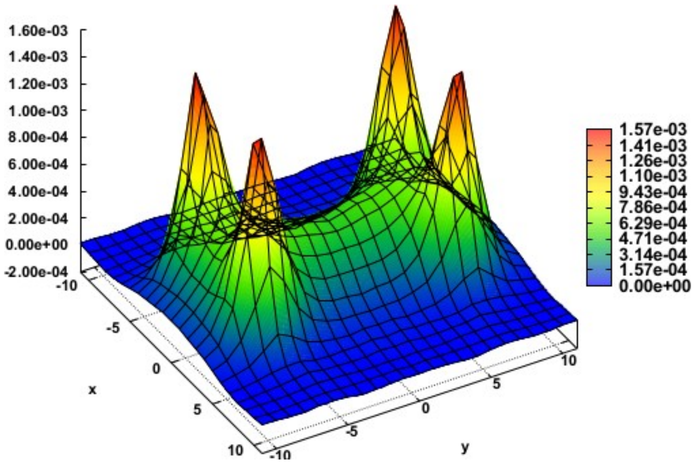

Fig. 2- 3D plot of Lagrangian density of the static tetraquark flux tube in the charges plane.

Selected references:

[1]- Colour Fields Computed in SU(3) Lattice QCD for the Static Tetraquark System, Nuno Cardoso, Marco Cardoso, Pedro Bicudo, Phys.Rev. D84, 054508 (2011)

[2]- u-d-bbar-bbar tetraquark resonances with lattice QCD potentials and the Born-Oppenheimer approximation, Pedro Bicudo, Marco Cardoso, Antje Peters, Martin Pflaumer, Marc Wagner, Phys.Rev. D96, 054510 (2017) :

News and Events

2018

Workshops

-First CeFEMA-IT Workshop on Quantum Technologies
March 1 2018
Physics Building IST

-Training School: NMR relaxometry for food and environmental applications. Eurelax Cost Action ca15209
14-16 February 2018
Physics Building IST

Seminars

The Manufacture of Mice: Where Organ Engineering Must Go
Edward Leonard
(Columbia University, USA)
June 4, 2018, South tower, IST

2019

Workshops' program;

One workshop per semester, organized alternatively by the two CeFEMA's nucleus.

Seminars' program;

A seminar every two weeks with alternating external and internal speakers.

Contacts

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