



CHAYENE GONÇALVES ANCHIETA

Curriculum Vitae

CURRENT ADDRESS

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PERSONAL

Born April 13, 1989 in Santana do Livramento, Brazil; married

Languages: English, Spanish, Portuguese. (Beginner in German)

EDUCATION

2015 - 2019 **Ph.D. in Chemical Engineering.**
Chemical Engineering Department, Federal University of São Carlos, UFSCAR, São Carlos, Brazil
Thesis: Ni catalysts supported over oxides synthesized using ionic liquids: Catalytic activity in tri-reforming of methane.
Supervisor: José Mansur Assaf
Fellowship: Conselho Nacional de Desenvolvimento Científico e Tecnológico - CNPq

2013 - 2015 **M.S. in Process Engineering.**
Chemical Engineering Department, Federal University of Santa Maria, UFSM, Santa Maria, Brazil
Thesis: Synthesis of zinc ferrite (ZnFe_2O_4) by different route and its catalytic activity in photo-Fenton reaction.
Supervisor: Edson Luiz Foletto
Fellowship: Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – CAPES

2012 - 2013 **Guest Student at Chemical Engineering Department**
Federal University of Santa Maria, UFSM, Santa Maria, Brazil

2006 - 2011 **BSc in Chemical Engineering.**
Federal University of Pampa, UNIPAMPA, Bage, Brazil
Dissertation: Use of rice husk ash as substitute for diatomaceous Earth in wine filtration process.
Supervisor: Sergio Meth

ACADEMIC AND PROFESSIONAL EXPERIENCE

November 2023

– Current

Invited Researcher.
Chemical Engineering School
University of Campinas, UNICAMP, Campinas, Brazil

November 2021

- January 2024 Postdoctoral Researcher.
microXAS beamline, Swiss Light Source SLS
Paul Scherrer Institut, PSI, Switzerland

October 2021

- October 2023 Invited Researcher.
Chemical Engineering School
University of Campinas, UNICAMP, Campinas, Brazil

April 2019

- October 2021 Postdoctoral Researcher.
Laboratory of Advanced Batteries
University of Campinas, UNICAMP, Campinas, Brazil
Chemical Engineering School

2015 - 2019

PhD Student.
Chemical Engineering Department
Federal University of São Carlos, UFSCAR, São Carlos, Brazil
Research Centre for Greenhouse Gas Innovation - project financed by Shell

2011 – 2012

Internship.
R&D: Filtration process and Filter media. Development of new filter, using of rice husk ash as substitute for diatomaceous Earth.
Almaden Winery – Miolo Wine Group Brazil

HONORS AND AWARDS

Inventors Award 2022, Licensed Technology, Innovation Agency of UNICAMP, University of Campinas.

RESEARCH PROJECTS

2023 - Current Hydrogen Production via Ammonia Reforming Over Ni-Based Catalysts in a Microchannel Reactor - University of Campinas, UNICAMP, Campinas, Brazil – FAPESP grant: *FAPESP 2015/20630-4 and 2022/16379-8*

The project aim is to explore and establish an efficient and novel method for hydrogen (H₂) production by reforming ammonia and ammonium hydroxide (NH₄OH) using microchannel reactors. Focused on addressing the challenges of current H₂ generation, particularly the environmental impact and high costs associated with traditional methods, the project aims to develop a scientifically innovative approach. Through a comprehensive study involving simulation and experimentation, the objective is to determine thermodynamic models, reaction kinetics, and optimal operating parameters for the reforming process. The project also involves the manufacturing and testing of microchannel reactors, incorporating 3D printing and Ni-based catalysts. Advanced in situ characterization techniques will be employed to enhance the understanding of catalyst behavior during the reforming reactions. The ultimate goal is to contribute valuable data to the scientific community and explore the potential for technology transfer to industries, offering a safer, more cost-effective, and environmentally friendly alternative for H₂ production.

2023 - Current Nanotechnology applied to the development of active materials for Li batteries with immediate and future impact. – Grant CNPq/MCTI N° 42/2022 - Support for Cooperative Projects in Nanotechnology within the Scope of the Brazilian-Argentine Center for Nanotechnology – CBAN.

The project involves advanced methodologies in the field of nanotechnology for the study of active materials in Li batteries, based on the experience and capacity of both participating groups. The materials to be studied range from cathodes used in batteries involving Li-ion technology, with immediate impact, to the development of new materials to be used in high energy density technologies such as Li-S and Li-air. There is complementarity between the groups for cooperation both in the methodologies adopted and in the study systems, synergistically expanding the groups' capabilities in both aspects. The interaction that each of the groups has with the productive sector stands out, supported by current agreements with technology-based companies, which makes the impact of proposed research and developments of concrete and specific interest, and allows natural feedback to define the problems to be studied from a realistic perspective. Regarding methodologies, the project addresses the use of traditional and advanced techniques, highly appropriate for the detailed chemical and structural study of active materials. The techniques will be based on the absorption of X-rays, adapted for the proposed "operando" studies during the charging and discharging processes, including, in some cases, spatial resolution on a nanometric scale. Own facilities are available for this in the Argentine group and in the synchrotron laboratories in Campinas.

2021 - 2024 In Operando investigation of bifunctional catalysts in Li-air Batteries. – Paul Scherrer Institut - PSI, Villigen, Switzerland

The project aims to develop a new cell for operando imaging characterization of batteries. The project also works on the development of NiO/ZrO₂ for Li-air batteries in order to improve the battery's capacity and life cycle under water contamination. Chemical imaging microanalysis combining XRD, XAS and XRF will allow the chemical, structural and redox state study of tetrahedral and octahedral sites of electrocatalysts.

2019 - 2023 Design and confection of new electrodes applied to Li-air. - Advanced Energy Storage – CINE/SHELL Center for Innovation on New Energy - University of Campinas, UNICAMP, Campinas, Brazil

The project aims to develop new electrodes to be applied as a cathode in Li-O₂ cells. The project also works on the development of redox mediators for O₂ reactions in order to improve the robustness of the electrode design. In-situ characterization techniques under real operating conditions, performed in a separate project, will also contribute to the development of new electrodes.

2019 - 2023 In situ characterization of Li-O₂ in dynamic operating conditions.- Advanced Energy Storage – CINE/SHELL Center for Innovation on New Energy - University of Campinas, UNICAMP, Campinas, Brazil

The project aims to develop new prototypes in Li-O₂ cells for in-situ characterization under real operating conditions. The combination of information between different techniques will allow a significant understanding of surface chemistry and the interaction of the species formed with the electrodes used.

2018 - 2023 Synthesis gas production by methane tri-reforming - RCGI - Research Gas Innovation – RCGI/SHELL- Federal University of São Carlos, UFSCAR, São Carlos, Brazil

The aim of this project is to use CH₄ and CO₂ as raw materials (chemistry of C1) to produce synthesis gas (H₂ + CO), including catalyst development, proof of concept and technological applications, design and optimization of processes. This project will develop a process called methane tri-reforming, in which water, CO₂ and O₂ are used to produce synthesis gas with H₂/CO ratio suitable for synthesis of fuels.

2012 - 2015 Zn₂SnO₄ ternary oxide utilization as photocatalyst for organic compounds degradation over solar irradiation - Federal University of Santa Maria, UFSM, Santa Maria, Brazil.

Semiconductors are able to degrade many organic compounds such as detergents, dyes, pesticides, and volatile components under UV irradiation. Several studies on catalytic photodegradation of dyes have been reported. Thus, search for new materials in heterogeneous photocatalysis with high performance has been the subject of interest in recent years. The general objective of this work is to evaluate the activity of zinc stannate in the degradation of organic compounds under solar irradiation.

RESEARCH ACTIVITIES

Energy Storage and Conversion Devices

Interested in different energy conversion and storage devices: reactors; reformers; SOFC; micro-channel reactors; ammonia reforming; hydrogen production; syngas; Lithium, Sulfur and Sodium batteries, Solid-State batteries and supercapacitors

Catalysts and Electrolyte Synthesis

Use different synthesis methods to tune materials physicochemical properties: hydrothermal, solvothermal; precipitation, sol gel, microwave-assisted, solid state, etc.

In situ and In Operando Synchrotron Characterization

Use in situ and in operando characterization to understand chemical, structural and morphologic changes under dynamic conditions.

Cell Design

Develop new cells and devices for in situ and in operando characterizations allowing different applications. Actual: 3D cell for imaging characterization: x-ray and neutrons characterization.

Electrode Development

Use different technologies to enhance the electrochemical properties of the oxide-based and carbon-based electrodes: spin coating, bucky paper, catalytic ink, chemical vapour deposition (CVD), self-standing.

SKILLS

Optimization: *Design of Experiments (DOE) for reactional process*

Characterizations: *Gas Chromatography (GC), Thermal Analysis (DSC, TGA), Temperature-Programed Desorption and Reduction (TPD and TPR), Infrared Spectroscopy (FTIR), X-ray absorption Spectroscopy (XAS), X-ray Diffraction (XRD), Microscopy (SEM, TEM, AFM), Raman Spectroscopy, X-ray Photoemission Spectroscopy (XPS), N₂ Physisorption, synchrotron and neutron characterizations*

Synthesis: *Hydrothermal, Solvothermal, Microwave-assisted, precipitation, co-precipitation, impregnation, coating, Chemical Vapor Deposition (CVD), complexation*

Materials: *Spinel, Perovskites, Mixed Metal Oxides, Ionic liquids, NiO, CeO₂, ZrO₂*

Chemical Process: *Heterogeneous Catalysis, Ammonia reforming, Reforming, Tri-reforming, syngas, hydrogen production, Wastewater Treatment, Advanced Oxidative Process, Photocatalysis, Electrocatalysis, Lithium batteries, Oxygen Reduction and Evolution reaction, Solid-State Battery.*

SPECIALIZED COURSES AND EVENTS ATTENDED

2022	HERCULES 2022 European School: Neutrons and Synchrotron Radiation for Science. ALBA, DESY, Elettra and FERMI, KIT, PSI and SOLEIL.
2020	2020 SSRL Synchrotron X-ray Absorption Spectroscopy Summer School. Stanford Synchrotron Radiation Lightsource, SSRL, Estados Unidos
2020	Machine Learning. University of Campinas, UNICAMP, Campinas, Brazil
2020	Gas Adsorption in porous media. Brazilian Catalysis Society, SBCAT, Rio De Janeiro, Brazil

- 2020** X-ray Diffraction and Pair Distribution Function Analysis.
Brazilian Catalysis Society, SBCAT, Rio De Janeiro, Brazil
- 2020** 2nd Dense Energy Carriers Workshop, UNICAMP, Brazil.
- 2020** V CINE-CMSC Workshop: Scientific Discussions from CH₄ Conversion to Machine Learning Applications, University of Sao Paulo - USP, Brazil.
- 2020** Novel chemical catalytic and photocatalytic processes for the direct conversion of methane and CO₂ to products, University of Sao Paulo - USP, Brazil.
- 2019** New Challenges and Approaches to Modern Catalysis.
Brazilian Catalysis Society, SBCAT, Rio De Janeiro, Brazil
- 2018** Continuous Chemical Methods: An Essential Set of Tools for Modern Synthesis.
Federal University of São Carlos, UFSCAR, Sao Carlos, Brazil
- 2018** Infrared Spectroscopy to Characterize Acid Active Sites.
University São Paulo, USP, Sao Paulo, Brazil
- 2018** LIGNIN-FIRST BIOREFINING: PAST, PRESENT AND FUTURE.
University of São Paulo, USP, Sao Paulo, Brazil
- 2017** Teaching Training.
Federal University of São Carlos, UFSCAR, Sao Carlos, Brazil
- 2016** Thermal Analysis.
Federal University of São Carlos, UFSCAR, Sao Carlos, Brazil
- 2014** Phase Equilibrium Engineering XX COBEQ 2014.
Brazilian Assosiation of Chemical Engineering, ABEQ, Sao Paulo, Brazil

LIST OF POTENTIAL REFERENCES

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Professor Dr. Marcio Antonio Mazutti

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LIST OF PUBLICATIONS

CHAYENE GONÇALVES ANCHIETA

Refereed Journal Articles

C. G. ANCHIETA, B. A. FRANCISCO, J. P. O. JÚLIO, P. TRTIK, A. BONNIN, G. DOUBEK, D. F. SANCHEZ. LiOH Decomposition by NiO/ZrO₂ in Li-Air Battery: Chemical Imaging with Operando Synchrotron Diffraction and Correlative Neutron/X-Ray Computed-Tomography Analysis. *Small Methods* 2024, 2301749. [doi:10.1002/smt.202301749]

ERIK ALVES, **CHAYENE G. ANCHIETA**, MANUEL PINZÓN, ANDRE MIRANDA, RODOLFO CASTANHO FERNANDES, FRANCISCO MAIA, CRISTIANE BARBIERI RODELLA, LEONARDO MORAES DA SILVA, GUSTAVO DOUBEK, HUDSON ZANIN. Combining in situ electrochemistry, operando FTIR and post-mortem analyses to understand Co-Mn-Al spinels on mitigating shuttle effect in lithium-sulfur battery. Just Accepted. Available online 20 August 2023. [doi: 10.1016/j.nanoen.2023.108809]

BRUNO A. B. FRANCISCO, JÚLIA P. O. JÚLIO, **CHAYENE G. ANCHIETA**, THAYANE C. M. NEPEL, RUBENS M. FILHO, GUSTAVO DOUBEK. Systematic study of O₂ supply in Li-O₂ batteries with high and low donor number solvents. *ACS Applied Energy Materials*, 2023. [doi: 10.1021/acsaem.3c00057].

POLICANO, MARTIM CHIQUETTO; **GONÇALVES ANCHIETA, CHAYENE**; CARPANEDO DE MORAIS NEPEL, THAYANE; CARLOS BARBOSA MAIA, FRANCISCO; Maciel Filho, Rubens; DOUBEK, GUSTAVO. The Double-Edged Effect of Water on Li-O₂ Aprotic Batteries. *JOURNAL OF THE ELECTROCHEMICAL SOCIETY*, 2023. [doi:10.1149/1945-7111/acc2ea]

LEAL SILVA, JEAN FELIPE ; POLICANO, MARTIM CHIQUETTO ; TONON, GIOVANA CHINAGLIA; **ANCHIETA, CHAYENE GONÇALVES** ; DOUBEK, GUSTAVO ; Maciel Filho, Rubens . The potential of hydrophobic membranes in enabling the operation of lithium-air batteries with ambient air. *Chemical Engineering Journal Advances*, 2022. [doi: 10.1016/j.cej.2022.100336]

MARTIM C. POLICANO, **CHAYENE G. ANCHIETA**, THAYANE C. M. NEPEL, GUSTAVO DOUBEK, RUBENS M. FILHO. Water in aprotic Li-O₂ batteries: A critical review. *ACS Applied Energy Materials*, 2022. [doi:10.1021/acsaem.1c03750].

TUANAN C. LOURENÇO, LETÍCIA M. S. BARROS, **CHAYENE G. ANCHIETA**, THAYANE C. M. NEPEL, JÚLIA P. O. JÚLIO, LUIS GUSTAVO DIAS, RUBENS MACIEL FILHO, GUSTAVO DOUBEK, AND JUAREZ L. F. DA SILVA. Tuning Aprotic Solvent Properties with Long Alkyl Chain Ionic Liquid for Lithium-based Electrolytes. *Journal of Materials Chemistry A*, 2022. [doi: 10.1039/D1TA10592B].

PATRÍCIA D. BOHN; **CHAYENE G. ANCHIETA**; KÁTIA R. KUHN, EDSON I. MULLER; FLÁVIO D. MAYER; RAQUEL C. KUHN. Conversion of rice husk into reducing sugars: influence of pretreatment with water and [C₁₆MIM][Br⁻] ionic liquid. *Clean Technologies and Environmental Policy*, 2022. [doi: 10.1007/s10098-022-02302-4].

JÚLIO, JÚLIA P.O.; FRANCISCO, BRUNO A.B.; DE SOUSA, BIANCA P.; SILVA, JEAN FELIPE LEAL; **ANCHIETA, CHAYENE G.**; NEPEL, THAYANE C. DE M.; RODELLA, CRISTIANE B.; FILHO, RUBENS M.; DOUBEK, GUSTAVO. Effect of O₂ flow in discharge products and performance of Li-O₂ batteries. *Chemical Engineering Journal Advances*, 2022. [doi: 10.1016/j.cej.2022.100271]

ANCHIETA, CHAYENE GONÇALVES; ASSAF, ELISABETE MOREIRA; ASSAF, JOSÉ MANSUR. Syngas production by methane tri-reforming: Effect of Ni/CeO₂ synthesis method on oxygen vacancies and coke formation. *Journal of CO₂ Utilization*, 2022. [doi:10.1016/j.jcou.2021.101853]

NEPEL, THAYANE C. M.; **ANCHIETA, CHAYENE G.**; CREMASCO, LETICIA F.; SOUSA, BIANCA P.; MIRANDA, ANDRÉ N.; OLIVEIRA, L. C. C. B.; FRANCISCO, B. A. B.; JULIO, J. P. O.; MAIA, F. C. B.; FREITAS, R. O.; RODELLA, CRISTIANE B.; MACIEL FILHO, R.; DOUBEK, G. In Situ Infrared Micro and Nanospectroscopy for Discharge Chemical Composition Investigation of Non-Aqueous Lithium–Air Cells. *Advanced Energy Materials*, 2021.

SILVA NETO, LUIZ D.; **ANCHIETA, CHAYENE G.**; DUARTE, JOSÉ L. S.; MEILI, LUCAS; FREIRE, JOSÉ T. Effect of Drying on the Fabrication of MgAl Layered Double Hydroxides. *ACS Omega*, 2021. [doi:10.1021/acsomega.1c03581]

CREMASCO, LETICIA F.; **ANCHIETA, CHAYENE G.**; NEPEL, THAYANE C. M.; MIRANDA, ANDRÉ N.; SOUSA, BIANCA P.; RODELLA, CRISTIANE B.; FILHO, RUBENS M.; DOUBEK, GUSTAVO. Operando Synchrotron XRD of Bromide Mediated Li-O₂ Battery. *ACS Applied Materials & Interfaces*, 2021. [doi:10.1021/acsaami.0c21791]

ANCHIETA, CHAYENE GONÇALVES; ASSAF, ELISABETE MOREIRA; ASSAF, JOSÉ MANSUR. Effect of ionic liquid in Ni/ZrO₂ catalysts applied to syngas production by methane tri-reforming. *INTERNATIONAL JOURNAL OF HYDROGEN ENERGY*, 2019.

SEVERO, E. D. C.; **ANCHIETA, C. G.**; FOLETTO, V. S.; KUHN, R. C.; COLLAZZO, G. C.; MAZUTTI, M. A.; FOLETTO, E. L. Degradation of Amaranth azo dye in water by heterogeneous photo-Fenton process using FeWO₄ catalyst prepared by microwave irradiation. *Water Science and Technology*, 2016. [doi:10.2166/wst.2015.469]

SEVERO, ERIC DA CRUZ; ABAIDE, EDERSON ROSSI; **ANCHIETA, CHAYENE GONÇALVES**; FOLETTO, VITÓRIA SEGABINAZZI; WEBER, CAROLINE TREVISAN; GARLET, TAIS BISOGNIN; COLLAZZO, GABRIELA CARVALHO; MAZUTTI, MARCIO ANTONIO; GÜNDEL, ANDRÉ; KUHN, RAQUEL CRISTINE; FOLETTO, EDSON LUIZ. Preparation of Zinc Tungstate (ZnWO₄) Particles by Solvo-hydrothermal Technique and their Application as Support for Inulinase Immobilization. *Materials Research (São Carlos. On-line)*, 2016. [doi:10.1590/1980-5373-mr-2015-0100]

ANCHIETA, C. G.; TOCHETTO, L.; MADALOSSO, H. B.; SULKOVSKI, R. D.; SERPA, C.; MAZUTTI, M. A.; ALMEIDA, A. R. F. DE; GÜNDEL, A.; FOLETTO, E. L. Effect of thermal treatment on the synthesis of NiAl₂O₄ spinel oxide using chitosan as precursor. *Ceramica*, 2015. [doi:10.1590/0366-69132015613601925]

ABAIDE, EDERSON ROSSI; **ANCHIETA, CHAYENE GONÇALVES**; FOLETTO, VITÓRIA SEGABINAZZI; REINEHR, BEATRIZ; NUNES, LUCIELLE FERREIRA; KUHN, RAQUEL CRISTINE; MAZUTTI, MARCIO ANTONIO; FOLETTO, EDSON LUIZ. Production of Copper and Cobalt Aluminate Spinel and Their Application As Supports for Inulinase Immobilization. *Materials Research*, 2015. [doi:10.1590/1516-1439.031415]

ANCHIETA, CHAYENE G.; SEVERO, ERIC C.; RIGO, CAROLINE; MAZUTTI, MARCIO A.; KUHN, RAQUEL C.; MULLER, EDSON I.; FLORES, ERICO M.M.; MOREIRA, REGINA F.P.M.; FOLETTO, EDSON L. Rapid and facile preparation of zinc ferrite (ZnFe₂O₄) oxide by microwave-solvothermal technique and its catalytic activity in heterogeneous photo-Fenton reaction. *Materials Chemistry and Physics*, 2015. [doi:10.1016/j.matchemphys.2015.04.016]

ANCHIETA, CHAYENE G.; DOTTO, GUILHERME L.; MAZUTTI, MARCIO A.; KUHN, RAQUEL C.; COLLAZZO, GABRIELA C.; CHIAVONE-FILHO, OSVALDO; FOLETTO, EDSON L. Statistical optimization of Reactive Red 141 removal by heterogeneous photo-Fenton reaction using ZnFe₂O₄ oxide prepared by microwave irradiation. *Desalination and Water Treatment (Print)*, 2015. [doi:10.1080/19443994.2015.1070761]

ANCHIETA, CHAYENE; CANCELIER, ADRIANO; MAZUTTI, MARCIO; JAHN, SÉRGIO; KUHN, RAQUEL; GÜNDEL, ANDRÉ; CHIAVONE-FILHO, OSVALDO; FOLETTO, EDSON. Effects of Solvent Diols on the Synthesis of ZnFe₂O₄ Particles and Their Use as Heterogeneous Photo-Fenton Catalysts. *Materials (Basel)*, 2014. [doi:10.3390/ma7096281]

ANCHIETA, CHAYENE G.; SALLET, DANIELA; FOLETTO, EDSON L.; DA SILVA, SYLLOS S.; CHIAVONE-FILHO, OSVALDO; DO NASCIMENTO, CLAUDIO A.O. Synthesis of ternary zinc spinel oxides and their application in the photodegradation of organic pollutant. *Ceramics International*, 2013. [doi:10.1016/j.ceramint.2013.08.074]

Review Articles and Reviewed Book Chapters

LORRANE C. C. B. OLIVEIRA, RAISSA VENÂNCIO, PAULO V. F. DE AZEVEDO, **CHAYENE G. ANCHIETA**, CRISTIANE B. RODELLA, HUDSON ZANIN, GUSTAVO DOUBEK. Reviewing oxide perovskite sites influence on electrocatalytic reactions for high energy density devices. Just Accepted - Journal of Energy Chemistry. 2023. [doi: 10.1016/j.jechem.2023.02.013]

LINO, A. P.; **ANCHIETA, CHAYENE GONÇALVES**; ASSAF, ELISABETE MOREIRA; ASSAF, JOSÉ MANSUR. Advances in Synthesis Gas Book Series. "Fuel gas production from syngas". Elsevier. Chapter 10, volume 3. ISBN: 9780323918787, 2022.

CANABARRO, NICHOLAS; SOARES, JULIANA F; **ANCHIETA, CHAYENE G**; KELLING, CAMILA S; MAZUTTI, MARCIO A. Thermochemical processes for biofuels production from biomass. Sustainable Chemical Processes. , v.1, p.22 - , 2013. [doi:10.1186/2043-7129-1-22]

Patents

ANCHIETA, C. G.; DOUBEK, G.; BARROS, L. M. S.; NEPEL, THAYANE C. M.; Maciel Filho, Rubens. ELECTROLYTE, BATTERIES INCLUDING A CRYSTALLINE IONIC LIQUID AS ADDITIVE IN ELECTROLYTE AND THE USE OF CRYSTALLINE IONIC LIQUID IN BATTERIES, 2021.

Category: Product. Institution where it was deposited: INPI - National Institute of Industrial Property. Country Brazil. Nature: Patent of Invention. Registration number: BR1020210169. Deposit date: 08/26/2021. Depositor/Holder: University of Campinas - UNICAMP. Licensed by Shell.

MIRANDA, A. N.; DOUBEK, G.; CREMASCO, L. F.; NEPEL, T. C. M.; **ANCHIETA, C. G.**; MACIEL FILHO, R. ELECTROCHEMICAL DEVICE FOR CHARACTERIZATION OF ELECTRODES IN DYNAMIC OPERATION REGIME, 2020.

Category: Product. Institution where it was deposited: INPI - National Institute of Industrial Property. Country Brazil. Nature: Patent of Invention. Registration number: BR10202002629. Deposit date: 12/21/2020. Depositor/Holder: UNICAMP Development Foundation.

Journal Articles in Preparation

CHAYENE G. ANCHIETA, BARTHÉLÉMY LELOTTE, HARI V. RAMASAMY, MARIO EL KAZZI, DARIO F. SANCHEZ. Unveiling He-Ncm(811) Transformations In Solid-State Batteries: Operando Chemical Imaging. Under preparation

BIANCA P. SOUSA, TUANAN C. LOURENÇO, **CHAYENE G. ANCHIETA**, JUAREZ L. F. DA SILVA, GUSTAVO DOUBEK. Direct Evidence of Reversible Changes in Electrolyte and its Interplay with LiO₂ Intermediate in Li-O₂ Batteries. Under review at Small.

BIANCA P. SOUSA, **CHAYENE G. ANCHIETA**, THAYANE M. C. NEPEL, ALEX R. NEALE, LAURENCE J. HARDWICK, RUBENS M. FILHO, GUSTAVO DOUBEK. Exploring Carbon Electrode Parameters in Li-O₂ Cells: Li₂O₂ and Li₂CO₃ Formation. Under review at Journal of Materials Chemistry A, published by the Royal Society of Chemistry

LETÍCIA M. S. BARROS, **CHAYENE G. ANCHIETA**, THAYANE C. M. NEPEL, JÚLIA P. O. JÚLIO, TUANAN C. LOURENÇO, LUIS GUSTAVO DIAS, RUBENS MACIEL FILHO, GUSTAVO DOUBEK, AND JUAREZ L. F. DA SILVA. Multifunctional Imidazolium-Based Ionic Liquid Crystal with Redox Mediator Properties for Li-O₂. Under preparation

Other Publications, Reports

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LIST OF NEUTRON AND SYNCHROTRON PROPOSALS

Accepted Proposals for Neutron Characterization

ANCHIETA, C. G.; PAVEL, T.; SANCHEZ, D. F. Proposal 20222518 - Tomographic Studies of NiO/ZrO₂ in Li-air Batteries at different stage of discharge and charge, 2023. NEUTRA beamline. The Swiss Spallation Neutron Source – SINQ. Switzerland. *High energy density devices are the future of energy storage. Lithium-Air batteries are one of the most promising candidates due to their high theoretical capacity. Monitoring the reactions and side product formation in Li-air batteries is crucial to develop a more stable device. The aim of this proposal is to understand the distribution of lithium species (LiOH, LiO₂ and Li₂O₂) and their evolution on the air electrode. The battery performance could be improved by understanding the air electrode, which is directly associated with applying mixed metal oxides in energy storage devices.*

Accepted Proposals for Synchrotron Characterization

ANCHIETA, C. G.; DOUBEK, G.; RODELLA, C. B. Proposal 20222009 - Defining the rigidity and mobility of structures of an ionic liquid crystal-based electrolyte for LiO₂ batteries via in situ XPCS, 2023. *Cateretê* beamline. Brazilian Synchrotron Light Laboratory – LNLS/Sirius. Brazil. *C₁₆mimBr is a multi-functional material with ionic liquid crystal character, forming micelles/ organized structures when dissolved in an aprotic electrolyte, and with redox mediator properties, reducing the cell charge overpotentials. The structure with nanodomains impacts the cell cyclability, so mobility and rigidity of those structures will be investigated through synchrotron in situ XPCS. Besides, USAXS will clarify the ions packaging and their size. Here, we propose a pioneer study using XPCS/USAXS to understand the role of C₁₆mimBr as an additive for Li-O₂ batteries.*

ANCHIETA, C. G.; SANCHEZ, D. F. Proposal 20222123 - X-ray Tomographic Studies of Mixed Metal Oxide in Li-air Battery at different stage of discharge and charge, 2023. cXAS beamline. Swiss Light Source – SLS. Switzerland. *The future of energy storage systems is directly related to devices with high energy density capacity. Lithium-Air batteries are one of the most promising candidates due to their high theoretical capacity. Therefore, a deeper understanding and monitoring the reactions and side products formation is crucial to develop a more stable device. The aim of this proposal is to understand the distribution of lithium species (LiOH, LiO₂ and Li₂O₂), the distribution NiO/ ZrO₂ catalysts, as well as the porous microstructure evolution on the air electrode. Understanding the air electrode which is direct associated to the battery performance will allow the application of mixed metal oxides in energy storage devices.*

ANCHIETA, C. G.; DOUBEK, G.; SANCHEZ, D. F. Proposal 20220536 - Operando Synchrotron X-ray Imaging Studies of Ni/ZrO₂ Mixed Metal Oxide in Li-metal Battery, 2022. microXAS beamline. Swiss Light Source – SLS. Switzerland.

Li-air batteries are promising candidates to be used as energy storage systems. This type of system has theoretical energy density capacity ten times higher than Li-ion battery. Design an efficient catalyst to be applied as air-electrode to enhance the kinetics of the oxygen reactions during the cycling processes involves a comprehensive and deep understanding of physico-chemical and structural properties. Thus, the aim of this proposal is to investigate the structural and chemical changes of Ni/ZrO₂, as a working electrode, under operating conditions and a full comprehension of the mechanism involved in their Li-air batteries cycling.

FREITAS, B. G. A.; ANCHIETA, C. G.; VICENTINI, R. F.; CARDENAS, M. J. P.; VENANCIO, R.; SANTOS, E. S.; RODELLA, C. B.; DOUBEK, G.; ZANIN, H. G.,. Proposal 20211035 - Synchrotron X-ray Diffraction Studies of metal oxides in Advanced Energy Storage Devices Under Operating Conditions, 2022. DanMAX beamline. MAXIV Laboratory. Sweden.

Pseudocapacitors are able to store Faradaic current through charge transfer between an electrode and an electrolyte. Metal oxides onto multi-walled carbon nanotube have been used as electrode material, due to its electrochemical and structural properties presented excellent results. Understanding the structural changes of LiCoO₂ during the operation process we will provide a deep understanding of the supercapacitor cycling processes.

FREITAS, B. G. A.; ANCHIETA, C. G.; VICENTINI, R. F.; CARDENAS, M. J. P.; VENANCIO, R.; SANTOS, E. S.; RODELLA, C. B.; DOUBEK, G.; ZANIN, H. G.,. Proposal 20220344 - Operando XANES Studies of the LiCoO₂

electrode in Supercapacitor, 2022. Carnauba beamline. Brazilian Synchrotron Light Source Laboratory – LNLS. Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil.

Supercapacitors are ultrafast energy storage devices. The ability of those devices to store energy is associated with the structure of the electrode and electrolytes interfaces. Metal oxides, such as LiCoO_2 , onto carbon nanotube have been used as electrode, due to excellent results. Therefore, we intend to examine the electrochemical and structural behavior of LiCoO_2 in the aqueous electrolyte.

NEPEL, T. C. M.; ANCHIETA, C. G.; POLICANO, M. D.; RODELLA, C. B.; DOUBEK, G. Proposal 20210226 - **Operando Characterization Of Li-O₂ Battery With Micro-Ftir**, 2022. Imbuia beamline. Brazilian Synchrotron Light Source Laboratory – LNLS. Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil.

The use of micro-FTIR and SINS technique applied to Li-O₂ batteries is an important novelty considering energy storage devices and electrolyte in one of the keys to booster the device performance. The proposal to IMBUIA aims to evaluate the influence of the electrolyte over Li-O₂ battery using micro-FTIR characterization and this proposal to LCTE is fundamental to prepare the samples.

NEPEL, T. C. M.; ANCHIETA, C. G.; POLICANO, M. D.; RODELLA, C. B.; DOUBEK, G. Proposal 20210119 - **Micro-Ftir Characterization Of Electrolyte For Lithium-Air Battery**, 2021. Imbuia beamline. Brazilian Synchrotron Light Source Laboratory – LNLS. Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil.

The use of micro-FTIR and SINS technique applied to Li-O₂ batteries is an important novelty considering energy storage devices. This proposal to IMBUIA aims to evaluate the influence of the electrode polarization over the infrared detection of Li-O₂ electrolyte using micro-FTIR characterization. The results are necessary to submit a complete answer for the reviewers of Advanced Energy Materials aiming the paper publication.

ANCHIETA, C. G.; SILVA, J. F. L.; RODELLA, C. B.; DOUBEK, G.; MACIEL FILHO, R. Proposal SEM-C1 - 26117 - **Morphologic Characterization Of Redox Mediator Based Lithium-Air Battery Electrodes**, 2020. Brazilian Nanotechnology National Laboratory- LNNano; Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil

ANCHIETA, C. G.; MIRANDA, A.N.; SILVA, J. F. L.; RODELLA, C. B.; DOUBEK, G. Proposal 20190057- **Operando Nano-Ftir Characterization Of Non-Aqueous Lithium-O₂ Cells**, 2019. IR beamline. Brazilian Synchrotron Light Source Laboratory – LNLS. Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil

By performing operando nano-FTIR characterization during typical cycling cells (Operando) we intend to investigate modifications on the surface along with changes of chemical composition of the system. Through the data given by the technique we aim to have deeper understanding of the processes that take place on the electrode surface (especially electrocatalysis and electrolyte degradation). This information will be relevant by allowing the scientific community to build a broader knowledge about the lithium-air system, aiding the development process for a practical cell.

CRUZ A. M.; ANCHIETA, C. G.; SILVA, A. H. M.; SANTANA, C. S.; GOMES, J. F.; ASSAF, J. M. Proposal 20180144 - **In-situ reduction of Cu-based materials**, 2018. XAFS2 beamline. Brazilian Synchrotron Light Source Laboratory – LNLS. Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil

CuO/CeO₂ catalysts have been extensively studied and are promising to be used in the COPROX reaction. Different synthesis methods of CuO/CeO₂ can lead to distinct dispersions of CuO on CeO₂, impacting directly on the CuO-CeO₂ interface and, consequently, the catalytic performance of these materials. The effects of the synthesis method of CuO/CeO₂ on their properties are still under debate in the literature. This knowledge is of fundamental importance to explain the catalytic process in the CO-PROX reaction. The in situ XAFS study could further clarify these effects on the materials redox behavior, through the investigation of electronic properties of the copper phase under reduction, oxidation and reaction conditions.

SILVA, A. H. M.; SANTANA, C. S.; ANCHIETA, C. G.; Cruz A. M.; GOMES, J. F.; ASSAF, J. M. Proposal 20180219 - **In-situ XRD study of Cu- and Pd - based catalysts applied to CO₂ hydrogenation**, 2018. XPD beamline. Brazilian Synchrotron Light Source Laboratory – LNLS. Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil

The catalytic conversion of CO₂ to fuels, as methanol for example, can contribute to the greenhouse gas mitigation and fossil fuels substitution. In the CO₂ to methanol reaction, Cu and Pd-based catalysts have been investigated. The addition of promoters into the catalyst formulation and the properties of the support were found to impact the catalytic performance of these materials. In this proposal, we intend to analyze a variety of Zn, Al, Cr, Ga and/or Zr containing Cu and Pd catalysts by in situ XRD in order to further clarify the changes in the Cu or Pd materials properties induced

by different supports or promoters and the effect of these modifications on the performance of these catalysts towards the CO₂ hydrogenation.

ANCHIETA, C. G.; Cruz A. M.; SANTANA, C. S.; GOMES, J. F.; ASSAF, JOSÉ MANSUR. Proposal 20180243 - **Investigation Of The Structure Of Ni/Zirconia Catalyst Prepared Via Ionothermal Route In Tri-Reforming Of Methane**, 2018. DXAS beamline. Brazilian Synchrotron Light Source Laboratory – LNLS. Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil

Nickel catalysts, have been regarded as the promising catalyst for tri-reforming of methane (TRM). However, the stability of nickel catalysts at high temperatures and the coke generation are the main obstacles for their applications. The nature of active site for TRM is driven by particle size and oxidation state. The ionic liquid adding to zirconia seems to change the interaction between nickel and support, resulting on different reduction temperatures of the samples as observed by temperature-programmed reduction with hydrogen (H₂-TPR) and preliminary in situ XRD and XANES results.

ANCHIETA, C. G.; LINO, A. V. P.; MARCOS, F. C. F.; ASSAF, J. M. Proposal 20170723 - **In-Situ XPD Study Of MgAl₂O₄ Supported Nickel Catalysts Applied To Tri-Reforming Of Methane**, 2017. XPD beamline. Brazilian Synchrotron Light Source Laboratory – LNLS. Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil

The in situ XPD will be used to study the effects of support MgAl₂O₄ and additives like ZrO₂, ZrO₂+CeO₂, ZrO₂+La₂O₃, ZrO₂+Y₂O₃ and ZrO₂+Sm₂O₃ on performance of nickel catalysts by monitoring nickel phase changes in the reducing atmosphere and reaction conditions. The in situ XPD patterns will be used to verify the nickel reducing ability on the support and the catalyst deactivation by oxidation of metallic Ni in Methane Tri-Reforming reaction and to collect information about active phase dispersion by monitoring the evolution of nickel crystallite size during activation and reaction.

ANCHIETA, C. G.; LINO, A. V. P.; MARCOS, F. C. F.; RAMON, A. P.; SILVA, T. L.; ASSAF, J. M. Proposal 20170828 - **In-Situ XAS Study Of MgAl₂O₄ Supported Nickel Catalysts Applied To Tri-Reforming Of Methane**, 2017. XAFS2 beamline. Brazilian Synchrotron Light Source Laboratory – LNLS. Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil

MgAl₂O₄ supported Ni catalysts are extensively applied to methane reforming reactions. The interaction between active phase and support together with the promoter is of fundamental importance to understand the catalytic process of Methane Tri-Reforming. XAS technique can probe the effects of this interaction in nickel catalysts supported on MgAl₂O₄, promoted with 12 wt % ZrO₂, 12 wt % ZrO₂+CeO₂, 12 wt % ZrO₂+La₂O₃, 11 wt % ZrO₂+Y₂O₃ and 12 wt % ZrO₂+Sm₂O₃.

ANCHIETA, C. G.; MARCOS, F. C. F.; ASSAF, J. M.; ASSAF, E.M. Proposal 20160772 - **In-Situ Xrd Study Of Co-MgAlO And Ni-MgAlO Catalysts Derived From Hydrotalcites**, 2016. XPD beamline. Brazilian Synchrotron Light Source Laboratory – LNLS. Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil

The interaction of the active phase, either Ni or Co, with the support or promoter is of fundamental importance to understand the catalytic process, given that different interactions can lead to different mechanisms. Samples of Ni-MgAlO and Co-MgAlO with different contents of Ni and Co and calcined at different temperatures and previously characterized by ex situ XRD, TGA, SEM, BET, metallic area and TPR will be monitored by the in situ XRD. It is expected that these analyses along with the previous characterizations and preliminary catalytic tests can help to get a better comprehension of the behavior of the phases and the active species in the catalytic processes.

ANCHIETA, C. G.; LINO, A. V. P.; MARCOS, F. C. F.; ASSAF, E.M.; ASSAF, J. M. Proposal 20160821 - **In-Situ XRD Study Of MgAl₂O₄ Supported Nickel Catalysts Applied To Tri-Reforming Of Methane**, 2016. XPD beamline. Brazilian Synchrotron Light Source Laboratory – LNLS. Brazilian Center of Research in Energy and Materials – CNPEM, Campinas, Brazil

Ni/MgAl₂O₄ catalysts are resistant to carbon deposition due to the strong interaction between nickel and the support. To assure the nickel reducibility cycle, catalysts should be promoted with ZrO₂ and rare earth oxides. In situ XRD can illustrate the effects of support promoters - ZrO₂, ZrO₂+CeO₂, ZrO₂+La₂O₃, ZrO₂+Y₂O₃ and ZrO₂+Sm₂O₃ - on CH₄ tri-reforming by tracking nickel phase changes in the reaction conditions.