

XXI B-MRS Meeting

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**B-MRS**  
Meeting  
October 1st to 5th



BRAZILIAN MATERIA  
RESEARCH SOCIET

**Maceió-AL, Bra**

**October 1<sup>st</sup> to 5<sup>th</sup>, 2023**

Booklet

Presentation  
Schedule

Mobile  
App

until April 17 <sup>th</sup> May 1 <sup>st</sup>  Submission of Abstracts	June 06 <sup>th</sup> June 25 <sup>th</sup>  Abstract status notification	until June 19 <sup>th</sup> June 29 <sup>nd</sup>  Submission of Revised Abstract	June 26 <sup>th</sup> July 07 <sup>th</sup>  Final Abstract Notificatio n	until July 26 <sup>th</sup>  Submission for Student Awards
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**Poster Printing Service**

Do you want to print your poster at the Conference?

Conexão Montagens e Eventos can do it!

Before the conference: the file (in pdf format) should be sent by email until September, 28th to - [sinalizacaoconexao@gmail.com](mailto:sinalizacaoconexao@gmail.com)

Amount R\$ 70.00 - payment via PIX. The poster will be available at the Poster Help Desk at the Conference on Monday morning, October 2nd - 9am.

### Request for resources from FAPESP

Researchers from the State of São Paulo (BR) might be eligible for financial support from FAPESP. More information in the link below.

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## Welcome

The **Brazilian Materials Research Society (B-MRS)** and the **Committee of the XXI B-MRS Meeting** invite the worldwide community of materials research to attend the 2023 Meeting to be held at the Ruth Cardoso Cultural and Exhibition Center in **Maceió-Alagoas, Brazil, October 1st to 5th, 2023.**

This traditional forum is dedicated to recent advances and perspectives in materials science and related technologies. It will be an excellent opportunity to bring together scientists, engineers and students from academy and industry to discuss the state of the art of Materials Science discoveries and perspectives.

Maceió is one of the main Brazilian capitals that has received many tourists mainly due to the receptivity of its inhabitants, the beaches with warm waters and extraordinary gastronomy. We very well welcome to Maceió. Do not miss this opportunity.

## Organizing Committee



**Carlos Jacinto da Silva**  
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Universidade Federal de Alagoas



**Mário Roberto Meneghetti**  
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Institute of Chemistry and  
Biotechnology, Universidade  
Federal de Alagoas

# Materials Design for Na-ion Batteries based on Computational Simulations

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Sodium-ion batteries hold great promise as energy storage devices, however, their effectiveness hinges on the diffusion of sodium cations in electrolytes and the sodiation mechanism in electrodes. Unfortunately, our current understanding of these atomic-level processes remains insufficient, primarily due to the large atomic radius of Na cations. In this presentation, we will discuss important results obtained by our research group in the last few years concerning Na-ion batteries using computational simulations, including molecular dynamics, density functional theory, and data mining techniques. Specifically, we will investigate Na-ion diffusion across various electrolytes and the sodiation mechanism within carbon-based materials. One of our noteworthy findings was the co-intercalation mechanism's existence in model carbon-based electrode morphologies, such as the stacking of graphene layers. We found that the interlayer distance has a direct impact on the co-intercalation behavior. Electrodes with an interlayer distance greater than that of graphite represent a viable approach to enhancing Na-ion intercalation. Additionally, we will discuss electrochemical stability windows for various combinations of cation and anion molecules based on density functional theory calculations. Overall, our research contributes to a better understanding of the fundamental processes in Na-ion batteries, which will be critical for improving their efficiency and enabling their widespread use.