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News

Fundamental Research

Surface, interface and materials science

Electrochemistry and corrosion

Mohammed Bin Jassar received the Yves Chauvin 2024 Thesis Prize during a ceremony held at IFPEN in Rueil Malmaison on November 21. This prize, which rewards an IFPEN doctoral student each year for the quality and originality of their research work, was awarded by the IFPEN Scientific Council.

His research aimed to improve understanding, through a molecular modeling approach, of the formation and growth of the so-called "Solid Electrolyte Interphase" (SEI) layer that forms at the electrode/electrolyte interface in lithium batteries. The growth of the SEI layer is considered to be the primary aging mechanism that leads to the gradual capacity loss of lithium-ion batteries.

Can you tell us a little about your background?

After completing high school in Yemen, I was awarded a scholarship to pursue a **Bachelor's degree in Chemical Engineering** at King Fahd University of Petroleum and Minerals in Saudi Arabia. During my studies, I spent one semester at the University of Florida in the United States as an exchange student. Following my Bachelor's, I was awarded an Erasmus Mundus scholarship to pursue **a Master's degree in Chemical Nano-engineering**, studying at Aix-Marseille University in France, Wroclaw University of Science and Technology in Poland, and the University of Rome Tor Vergata in Italy.

During my Master's studies, I developed a strong interest in molecular modeling and electrochemistry, particularly in the context of batteries for energy storage. With the growing demand for energy transition technologies, the need for batteries with better performance, enhanced safety, and longer lifespan has become increasingly critical. Motivated by these challenges, I pursued a PhD through a CIFRE program, collaborating with Stellantis, ENS Lyon, and IFP Energies Nouvelles (IFPEN). My PhD research focuses on **the molecular modeling of the solid electrolyte interphase (SEI) in lithium batteries**.

What are you doing now?

I am currently pursuing a postdoctoral position at the École Normale Supérieure (ENS), Paris Sciences et Lettres (PSL) University. In this role, I am working on molecular modeling for electrochemical systems, with a particular focus on **the effect of solvation at the electrode interface** . My goal is to understand and **optimize the various processes occurring at these interfaces**, which not only enhances the performance of various electrochemical systems but also supports **key reactions, such as CO_2 and N_2 reduction**, which are crucial for the energy transition.

Can you give us some cues about the objective of your thesis research and its applications?

I built a molecular model combining quantum and classical methods to simulate **the growth of the SEI layer in lithium batteries** which is the primary aging mechanism leading to **capacity loss and the failure of battery performance**. This model provides a detailed atomistic view, enabling long-term performance predictions from short-term simulations. The model aligns well with experimental data, especially in **predicting the structure of the SEI and the behavior of capacity loss over time** , achieving in few days what would traditionally take months/years to study experimentally.

I have also addressed the challenges facing computational studies aimed at accelerating the development of better batteries by investigating the effects of various electrolyte species, such as solvents, salts, and additives. These effects play a crucial role in guiding the design of more efficient and reliable batteries. Specifically, I have evaluated the performance of computationally low-cost molecular methods, including electronic structure methods and classical force fields, to model the complex molecular behaviors of the SEI layer. Additionally, I have explored the challenges faced by newer approaches, such as machine learning-based methods.

The outcomes of the thesis are highly relevant to Battery Management Systems (BMS) used in various industries, such as electric vehicles, as well as in devices like laptops and cell phones, where they help manage battery health and enhance performance. Additionally, the methodologies and models developed in this thesis have applications beyond battery technology, as they can be adapted to other fields involving surface growth, such as corrosion and coating processes.

Could you give us some details about how you managed to share your time between ENS Lyon, Stellantis and IFPEN?

I spent the first part of my thesis at ENS Lyon, where I focused on acquiring fundamental knowledge in quantum mechanics. This provided me with the theoretical framework necessary for my research. After that, I moved to IFPEN in Rueil-Malmaison, where I spent the remaining time of my PhD. At IFPEN, I continued to explore quantum mechanical approaches while integrating them with classical methods to address challenges in SEI growth modeling. The goal was to combine both quantum and classical techniques to create more effective models that could better simulate battery behavior. Throughout the entire three-year period, I was in constant communication with battery experts at Stellantis. These meetings allowed me to share my progress and gain insights into the specific challenges primarily faced by the electric vehicle battery industry, enabling me to align my research with real-world industry needs. This collaboration between IFPEN, ENS Lyon and Stellantis was incredibly rewarding as it provided me with the opportunity to view my PhD from multiple perspectives: scientific, engineering, industrial, and economic.

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