14thAnnual International Conference on Industrial Engineering and Operations Management
Dubai, United Arab Emirates (UAE), February 12-14, 2024
Publisher: IEOM Society International, USA
Published: February 12, 2024 DOI: 10.46254/AN14.20240437

Accelerating Sodium-Ion Electrode Material Development Through Artificial Intelligence

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Abstract

Rechargeable batteries have proven to be the most efficient energy storage solution for the intermittent renewable energy sources. Currently, the lithium-ion battery (LIB) is regarded as the leading energy storage system because of its power and energy density. Nevertheless, LIBs are facing issues such as the limited availability of lithium precursor materials and the cost attributed to this issue. Thus, sodium ion batteries (SIBs) are regarded as a highly promising alternative to LIBs, but they are still under research. Battery research and especially battery material design is challenging because of the complex structure-property relationships, where different materials interact unpredictably and uncontrollably. Hence, artificial intelligence (AI) can be used to accelerate the process of battery electrode material discovery. There are many parameters that determine whether the battery electrode material is suitable or not, such as the voltage and the specific capacity which both contribute to the overall energy density. Additionally, the volume change throughout the cycles contribute to the safety, efficiency and cyclability of the battery. Thus, several AI techniques such as decision trees, support vector machine, random forest and deep neural network (DNN) models have been used to predict the average voltage, maximum specific capacity, and volume change of the battery. The results showed that the DNN model performed best with an average mean absolute error of around 0.164. Based on the results obtained, machine learning has proven to be a crucial tool towards revolutionizing the battery material industry.

Keywords
Artificial Intelligence, Electrode materials, Machine learning, Materials discovery, and Sodium ion batteries.

Biographies

Sara A. Alzaabi is a driven Chemical Engineer specializing in AI, currently pursuing a Masters in Water and Environmental Engineering at Khalifa University, Abu Dhabi. With a stellar academic background, Sara's research focuses on leveraging AI to accelerate Sodium Ion Batteries development. Her commitment to innovation is evident through winning first place in the 2022 and 2023 Undergraduate Research competitions for projects in green hydrogen production and AI-driven SQL query generation.

Ali Elkamel is a Full Professor of Chemical Engineering. He is also cross appointed in Systems Design Engineering. He holds a BSc in Chemical Engineering and BSc in Mathematics from Colorado School of Mines, MSc in Chemical Engineering from the University of Colorado, and PhD in Chemical Engineering from Purdue University. His specific research interests are in computer-aided modeling, optimization, and simulation with applications to energy planning, sustainable operations, and product design. Among his accomplishments are the Research Excellence Award, the Excellence in Graduate Supervision Award, the Outstanding Faculty Award, and IEOM Awards. He has more than 425 journal articles, 175 proceedings, and 50 book chapters. He is also a co-author of six books.

Georgios Karanikolos is currently an Associate Professor in Chemical Engineering at the University of Patras and visiting faculty at the Institute of Chemical Engineering Sciences (FORTH/ICE-HT), Greece. His was an Assistant and then Associate Professor of Chemical Engineering at Khalifa University since 2013. Prior to that, he was Postdoctoral Fellow at the University of Minnesota, and then a Marie Curie fellow at the Demokritos National Research Center in Athens. He is recipient of the Abu Dhabi Department of Education and Knowledge Award for Research Excellence (2018) and the 2019 Khalifa University Research Excellence Award.

Ali AlHammadi received his BSc in Chemical Engineering (CE) from the Petroleum Institute, Abu Dhabi (honors with distinction, 2011) and received his PhD from the Department of Chemical and Biomolecular Engineering (CHBE) at Rice University, Houston, TX, USA (2016). He is alumni of the Mohammed Bin Rashid Impactful Leadership Program and received numerous awards including Innovators Under 35 and Best Teacher Award.