Seminar

Thursday, May 18th, 2023
4 pm (Msk)

Modeling of Li-ion and post-Li-ion batteries: what can we learn at different scales?

Ezequiel Leiva

Facultad de Ciencias Quíimicas –
Universidad Nacional de Córdoba –
Argentina

Instituto de Investigaciones
en Fisico – Química de Córdoba,
CONICET-UNC – Argentina

Seminar

Broadcast

Speaker introduction

Ezequiel Leiva currently works at the Department of Theoretical and Computational Chemistry of the Faculty of Chemical Sciences (FCQ), National University of Córdoba (UNC), Argentina. He also belongs to the Instituto de Investigaciones en Físico-Química de Córdoba (Consejo Nacional de Investigaciones Científicas y Técnicas, CONICET). Ezequiel graduated from the University of Córdoba (PhD. 1982) and after postdocs in Germany (DAAD and Alexander von Humboldt Fellowships) and the USA in the field of theoretical electrochemistry, he obtained a full professorship at UNC. He is currently Senior Researcher at CONICET. In 2008, he led a project that led to the installation of the fastest supercomputer in Argentina, dedicated to nanoscience simulations. In 2013 he moved his focus of interest to Li-ion batteries and was one of the founders of the UNC Sustainable Energy Laboratory, with more than 30 researchers (http://www.laesunc.com/laes/). He is now operating there as a project manager. In 2019 he became a member of the National Academy of Sciences of Argentina. Ezequiel's current research projects involve experimental and theoretical work in the field of advanced materials for lithium-ion batteries and post-lithium technologies. Ezequiel has published more than 200 articles and 1 patent. The grants he has received exceed US$2,000,000.

Seminar abstract

At present, lithium-ion batteries have successfully established themselves as energy carriers for portable electronic devices, electric vehicles, and stationary storage. However, there is a growing demand for performance improvement, and the key factors that govern it are not fully understood. In particular, a proper description of lithium-ion intercalation in nanometer-sized materials is of paramount importance for battery electrode design to discover how size and geometry affect performance rate and lifetime.
In the present talk, we address the insertion of Li-ion into prototype anode and cathode materials through computer simulations. We will describe the use of kinetic Monte Carlo (kMC) simulations to analyze the dynamic behavior of lithium storage in graphite, in close comparison with experiments using different electrochemical techniques. On the other hand, we address the single-particle behavior for Li+ intercalation in nanometer- to microscopic-sized materials by numerical simulations, using a continuum model. We will also discuss the application density-functional calculations to post-lithium ion systems, such as Li-S.

Skoltech