MRS-T 中國材料科學學會
Materials Research Society-Taiwan

Invited speaker's information form of IUMRS-ICA 2017

Presentation on Symposium F2:
Materials Design, Discovery, and Optimization Based on Computation

Photo

Presentation title

Combining First-principle Calculations and Artificial Neural Network for Additive Screening in Lithium-ion Battery

Speaker's name and affiliation
Wen-Dung Hsu
Department of Materials Science and Engineering, National Cheng Kung University

City/ Country
Tainan, Taiwan

Email
wendung@mail.ncku.edu.tw

Brief biography of Speaker:

Dr. Wen-Dung Hsu is currently an associate professor in the department of materials science and engineering, National Cheng Kung University. His expertise is utilizing computational materials science methods including first-principle calculations, molecular dynamics simulations, Monte-carlo methods, and finite-element methods to study materials issues. His research interests are mechanical properties of materials from atomic to macro scale, lithium-ion battery, solid-oxide fuel cell, ferroelectrics, solid catalyst design for biodiesel, and processing design for single-crystal growth. He obtained his Ph. D. degree from the department of materials science and engineering, University of Florida in 2007. He then served as a Post-doc researcher in the department of mechanical engineering at University of Michigan. He has joined National Cheng Kung University since 2008.

Abstract:
Nowadays, a great deal of research regarding energy density and voltage of lithium ion batteries (LIBs) are being developed for applications in electric vehicles, mobile devices and large power equipment. However, cycling performance and safety in LIBs makes it crucially for the applications mentioned above. One way to address the issue is to stabilize the electrolytes using various solvent formulas and functional additives. The selection of the best additive among phosphides, sulfonate esters and lactam, etc., which perfectly fits the electrodes, can accelerate and improve the developments in LIBs. Our studies have demonstrated that the required properties to be a good additive candidate are prior reduction or oxidation than electrolyte, non-dissociation of additives after its reduction or oxidation and reduced or oxided products are easy to aggregate. Base on the acknowledgment of the requirements we have found the strong correlation between reduction potentials (RPs) and lowest unoccupied molecular orbital (LUMO) as well as oxidation potentials (OPs) and highest occupied molecular orbital (HOMO). In addition, from the view point of calculation it is much faster and easier to calculate LUMO and HOMO than to calculate RP and OP. Thus artificial neural network was adopted to find the transform matrices between molecular structure descriptors and LUMO or HOMO. The predicted LUMO and HOMO then used to calculation RP and OP by the correlation relation. The results show that around 80% accuracy can be achieved when compared to all first-principle calculations. The calculation cost, however, is only less than 1%. This demonstrates that the combining method is a promising method for fast additive screening.