Asian Consortium on Computational Materials Science (ACCMS) Centre
SRM University-AP, Amaravati, Andhra Pradesh, India
Webinar-35

Title: Charge Carriers in Mott Insulators : Testing the Limits of First Principles Theory

Abstract

Mott insulators remain one of the major challenges for density-functional calculations. Recent works by Zunger and coworkers have demonstrated that, qualitatively correct gapping of prototype Mott insulators, such as NiO, MnO, FeO, or CoO can be described by density-functional calculations, even for their paramagnetic phases using so called polymorphous band theory. The question that remains is, whether or not charge carriers introduced into these systems e.g. by defect doping can be correctly described using the same methods. We develop a self-interaction correction that correctly describes both localized and delocalized charge carriers. As I will show, our method recovers several hallmark features of Mott insulators, such as the split-off states that accompany localized gap states, as well as activation barriers for hopping of the localized carriers.

Short Biography

Prof. Raebiger obtained his D.Sc. degree from the Helsinki University of Technology in 2006, and moved on to work as a postdoc with Prof. Alex Zunger at the National Renewable Energy Laboratory in Golden, CO. He joined the faculty of Engineering Science at the Yokohama National University in 2008 as Assistant Professor, was promoted as Associate Professor in 2014, and Full Professor in 2024. In 2014-15, Prof Raebiger spent one year as a visiting professor at the Federal University of the ABC Region in Brazil. His research topics include theory of defects in semiconductors and insulators, transition metal compounds, theory of magnetism, quantum materials, 1D and 2D materials, as well as various flavors of electron correlations. He was awarded the J. W. Corbett Prize in 2005, the Encouragement of Research in Materials Science Award at IUMRS-ICEM in 2012, and a Contribution Award of the MRS-J in 2019.

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