FAKULTÄT FÜR CHEMIE

universität wien

Einladung zum Vortrag von

Doz. Dr. Vitaliy Romaka
Department of Materials Science and Engineering,
Lviv Polytechnic National University, Lviv, Ukraine

„DFT modeling of Half-Heusler and Heusler phases for Thermoelectric Application"

The complex utilization of different DFT methods allows predicting the main thermoelectric properties of half-Heusler and Heusler materials. They could be used to precisely refine their real crystal structure, to define the solubility limits of substitutional and interstitial solid solutions and evaluate their thermodynamic stability, to predict the behavior of resistivity and Seebeck coefficient, to explore the effects of structural disorder and to show peculiarities in chemical bonding. Combination of theoretical DFT methods with experimental techniques gives the key for better understanding the nature of thermoelectric phenomena in half-Heusler and Heusler materials.

Freitag, 28. Oktober 2016, 15:00 Uhr
Hörsaal 4, Währinger Straße 42, 1090 Wien

Alexander Bismarck
Institut für Materialchemie

Peter Franz Rogl
Institut für Physikalische Chemie

Bernhard Keppler
Dekan

Lothar Brecker
Vizedekan

Veronika Somoza
Vizedekanin