FAKULTÄT FÜR CHEMIE

universität wien

Einladung zum Vortrag von

Dr. Jana Pavlu

Department of Chemistry, Masaryk University, Brno, CZ

“Multiscale Modelling of Intermetallic Phases”

There is no doubt that materials and their development are essential for the evolution of the society we live in. During the last century, the achievements in electronic science, computer technology etc. have opened up enormous possibilities for progress in theoretical approaches working on different scale and leading to research and development of more sophisticated materials. Most, if not all, of properties of solids can be described by methods based on various principles and laws of physical chemistry such as quantum mechanics in nano-scale modelling and thermodynamics applied to CALPHAD approach (Computer Coupling of Phase Diagrams and Thermochemistry), which works on macroscopic level. This lecture presents the principles and possibilities of modelling of physical and chemical properties (crystallographic structure, magnetism, lattice stability, Gibbs energy, and enthalpy) of solid phases using both above mentioned approaches. It shows how that their cooperation contributes to understanding and prediction of the physical and chemical properties of materials.

Freitag, 11. Mai 2018, 15:15 Uhr
Seminarraum 2 der Fakultät für Chemie
Währinger Straße 42, 1090 Wien

Freddy Kleitz
Institut für Anorganische Chemie – Funktionelle Materialien

Veronika Somoza Vizedekanin	Bernhard Keppler Dekan	Lothar Brecker Vizedekan