FAKULTÄT FÜR CHEMIE

universität wien

Einladung zum Vortrag von

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„Phase diagrams and thermodynamics for material applications"

Materials are at the core of the functioning of modern technology, whether in energy and data storage, catalysis or simply in building a bridge from steel. Often very fundamental properties decide over a material's suitability for a certain application, such as its composition and its thermodynamic properties. This situation increases in complexity when different materials are joined or converted in a process and undergo a chemical reaction to form new compounds.
The required basic properties can be read from the phase diagram, which depicts the stability of phases with respect to composition, temperature, pressure, etc. It can also give a first forecast about possible chemical reactions between dissimilar materials, i.e. the formation of new phases that might have positive or detrimental properties (e.g. a lower melting point, low mechanical strength, high volume change). Phase diagrams are therefore indispensable for systematic materials and process design.
Although phase diagrams are typically first investigated through experiments, their computational modeling in combination with thermodynamics (CALPHAD) is gaining importance fast, in particular in integrated computational materials engineering. This approach allows to access phase diagram and thermodynamic data quickly, to predict material behavior under user chosen conditions and to modify these parameters without resource intensive further experimental work.
Besides a short introduction into reading simple phase diagrams, specific examples from the fields of molten oxides and metallic alloys for electronics, high temperature processes and energy storage will be given. These will demonstrate the versatility of these tools in determining application limits e.g. through melting points, material transformations and compositional restrictions, in the modeling of the chemical driving force that governs application and manufacturing processes and in giving an indication in what direction a reaction underlying an industrial process will proceed.

Freitag, 12. Mai 2017, 15:00 Uhr
Seminarraum 2
Währinger Straße 42, 1090 Wien

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Freddy Kleitz, Klaus Richter, Hans Flandorfer –
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