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HoMMage

Hysteresis Design of Magnetic Materials for Efficient Energy Conversion

Tuesday, 26 Jan. 2021, 9:00 s.t., TU Darmstadt, Zoom

Prof. Dr. Levente Vitos

Department of Materials Science and Engineering (MSE)

KTH Stockholm

Zoom information: Meeting-ID: 826 3326 5664
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Quantum mechanical modeling of chemically and magnetically complex alloys

Abstract:

Modern materials research receives increasing support from first-principles modeling based on Density Functional Theory (DFT). Such approach gives fundamental understanding, offers efficient pre-screening against various degrees of freedom and provides information where experimental assessments are limited or not feasible. Today the *ab initio* theory aided materials assay finds its way in almost all areas of advanced materials design and characterization.

Due to the complexity of the problem, DFT modeling was practically missing within the exciting field of multicomponent alloys such as stainless steels or high entropy alloys. Starting from 2000s, we made a series of attempts to fill this gap and extend the scope of *ab initio* modeling to high-technology alloys. In my seminar, I will overview the pioneering applications of alloy theory in the case of chemically and magnetically complex alloys, and point out the main known and hidden challenges associated with such efforts. I will present our theoretical predictions for the structural and magnetic properties of selected transition metal alloys. In particular, I will discuss our results obtained for the FeNi system as promising rare-earth free permanent magnet. Furthermore, I will present results on the plastic deformation mechanism in close packed metals and alloys. Finally, I will briefly discuss the possibility of metastable twinning in some special multicomponent alloys.

About the speaker:

Levente Vitos received PhD in solid state physics, Hungary 1997. He was postdoc at the Danish Technical University, Uppsala University and Royal Institute of Technology (KTH). Since 2000, he works at the Department of Materials Science and Engineering (MSE), KTH. In year 2005, he was appointed guest professor and in 2009 full professor in Computational Materials Design. In 2012, he took over the Applied Materials Physics group working with ab initio modeling of materials. Since 2015, he is the head of the Unit of Properties at MSE. His expertise includes Density Functional Theory, computational alloy theory, and materials modeling from first-principles. Together with his colleagues, he performed the first *ab initio* description of steels and high-entropy alloys; created databases for surface parameters of metals; and worked out the theory of plasticity for austenitic phase. He created the EMTO computational method, today used by more than 300 groups around the world.