

European XFEL Theory Seminar



Thursday, 13th of September 2018, 16:00
Campus Schenefeld, main building (XHQ) room E1.041

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Realistic description of strong correlations in solids and alloys

Engineering novel materials with specific electronic, magnetic, optical or transport properties is a challenge for material science. It relies crucially on our understanding of the underlying physical mechanisms. Increasing our knowledge about electronic and magnetic properties of materials has thus immediate impact onto possible technological advances. The DFT+DMFT approach, which is a combination of the Dynamical Mean Field Theory and the Density Functional Theory is a powerful tool to study from first principles the magnetic and electronic properties of strongly correlated compounds. Success application of the DFT+DMFT theory for a description of the physical properties of Invar and FeO₂H_x will be presented.

■ Host: Evgeny Gorelov