INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

Monday, 11th of April, 4:30 p.m.
ICAMS Seminar room UHW 11/1102

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## Material design for energy applications

Heusler compounds are a remarkable class of intermetallic compounds, exhibiting properties such as half-metallic ferromagnetism, superconductivity and semiconductance. The latte one is simply connected to the number of valence electrons. Their band gaps can easily be tuned from zero to $\approx$ 4eV by changing the chemical composition. Thus, great interest has been attracted in the fields of thermoelectrics, solar cells and diluted magnetic semiconductors. The combination of different properties leads to new multifunctional materials, which will revolutionize technological applications. This talk will give an overview about the structure, the origin of the band gap and the functionalities of semiconducting Heusler compounds and how to design materials for a particular application.