



INTERDISCIPLINARY CENTRE FOR  
ADVANCED MATERIALS SIMULATION

Monday, 15th of November, 4:30 p.m.  
ICAMS Seminar room UHW 11/1102

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## **Optimizing electronic properties of metal and semiconductor alloys using DFT + cluster expansion**

Demands for materials with peculiar properties, e.g. in magneto-electronics or photo-voltaics, call for quantum-mechanical modeling of complex atomic structures. Here we employ density-functional (DFT) calculations in combination with the cluster expansion (CE) of motifs on a lattice to bridge the gap between macroscopic properties and the atomic structure of alloys. Two examples:

Magnetic memory devices exploiting the tunneling magneto-resistance (TMR) effect depend crucially on the spin polarization of the electrodes. Some Heusler alloys, e.g.  $Co_2MnSi$ , if perfectly ordered, are ferromagnetic half-metals with (ideally) 100% spin polarization. In practice, however, their performance is limited by atomic disorder and deviations from perfect stoichiometry, but also by interface states at the tunneling barrier. We use ab initio thermodynamics in conjunction with CE to show that excess manganese, both in the alloy and at the interface, helps to preserve the desired half-metallic property.

In thin-film solar cells with  $CuIn_xGa_{1-x}Se_2$  absorber, the efficiency is limited by the homogeneity of the alloy. We use Metropolis Monte Carlo simulations employing a DFT-based CE to show that annealing at temperatures above 400 K is required to induce entropic mixing of In and Ga. Ga-rich alloys, while showing a good match of their band gap to the solar spectrum, are more prone to segregation, which presently limits their efficient use in solar cells.