# Electronic Correlations in the Optical Spectra of the CrMnFeCoNi High-Entropy Alloy

David Redka[1,3,a)], Andreas Held[2], Hubert Ebert[2], Heinz P. Huber[1] and Ján Minár[3]

[1]*Department of Applied Sciences and Mechatronics, Hochschule München, University of Applied Sciences, 80335 Munich, Germany*
[2]*Department of Chemie, Ludwig-Maximilians-Universit¨at München, 81377 Munich, Germany*
[3]*New Technologies-Research Center, University of West Bohemia, 30100 Plzen, Czech Republic*

[a)] Corresponding address: dredka@hm.edu; david_sebastian.redka@hm.edu

**Abstract**. High entropy alloys (HEA) are an emerging class of materials with promising and exciting properties for advanced future applications. Next to the primarily investigated outstanding mechanical properties, electronic structure and transport properties are of great interest, for both technology and basic science. In this regard, the analysis of photoemission and optical spectra is interesting, as these methods probe the electronic structure in a dynamic manner. To this end, we calculate the optical conductivity tensor of the CrMnFeCoNi HEA utilizing the fully relativistic SPRKKR band structure package [1,2] and compare the results to experimental data. Our approach is based on Kubo's linear response formalism for the current density response to an external perturbing electric field. In addition, we consider electronic correlation effects which go beyond the single-particle approximation of density functional theory by including dynamic mean-field calculations (DMFT) [3]. It is well known that DMFT is key to understand strongly correlated 3d transition metals, as seen in the photoemission spectra of Ni [3]. Our DMFT results and the analysis of the imaginary part of the self-energy are in good agreement with literature data on pure elements. Optical spectra up to 8 eV are calculated and discussed for different scenarios. We show that the use of DMFT significantly improves the calculations, especially in the interband transition dominated region of the optical spectrum above 1 eV. The optical conductivity we obtain is in excellent agreement with ellipsometric measurements made at room temperature. A reflectance variation of less than 5% could be attained across the whole spectral range.

1. H. Ebert, D. Ködderitzsch, and J. Minár, Calculating Condensed Matter Properties Using the KKR Green's Function Method—Recent Developments and Applications, Reports on Progress in Physics **74**, 096501 (2011)
2. T. Huhne and H. Ebert, Fully Relativistic Description of the Magneto-Optical Properties of Arbitrary Layered Systems, Phys. Rev. B **60**, 12982 (1999)
3. J. Minar, Correlation Effects in Transition Metals and Their Alloys Studied Using the Fully Self- Consistent KKR-Based LSDA + DMFT Scheme, Journal of Physics Condensed Matter 23, (2011)