TECHNISCHE UNIVERSITÄT WIEN
Vienna University of Technology

INSTITUT FÜR FESTKÖRPERPHYSIK
Institute of Solid State Physics

Wiedner Hauptstraße 8-10/138, 1040 Wien, AUSTRIA – T: +43-1-5880113801 / F: +43-1-5880113899 – E: sekretariat@ifp.tuwien.ac.at

# EINLADUNG zum IFP-SEMINAR

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| Thema: | **Impact of electronic correlation effects on thermoelectricity and the colour of materials** |
| Vortragender: | **Jan Tomczak**<br>Institut für Festkörperphysik, TU Wien |
| Host: | Karsten Held |
| Termin: | **Mittwoch, 26. Juni 2013, 16:00 Uhr** |
| Ort: | Institut für Festkörperphysik, TU Wien<br>Wiedner Hauptstraße 8-10, 1040 Wien<br>Seminarraum 138B, 7. OG (rote Leitfarbe) |
| Förderer: | ERC Ab Initio DGA |

**Abstract:**

In the first part of my talk I will present some of my recent efforts towards the understanding of correlated narrow-gap semiconductors, such as FeSi, $FeSb_2$, or $FeGa_3$. This class of materials received a lot of attention because its members exhibit large thermopowers, as well as striking similarities to heavy fermion Kondo insulators. Here, I will first review a coherence-decoherence scenario that I developed for FeSi. The methodology, that foots of realistic many-body calculations, accounts for all major observed anomalies: the metallization crossover, the lack of conservation of spectral weight in optical spectroscopy, and the Curie susceptibility. In particular, I will discuss the implications for the Seebeck coefficient. I will also show results for the thermoelectricity of other correlated semiconductors and will motivate that there is an upper bound for purely electronic contributions to the thermopower.

In the second part of my talk, I will discuss cerium fluorosulfide, CeSF, which is a brilliant red pigment. Despite its commercial use, the origin of its absorption properties were not understood, largely because band theory cannot describe the Mott physics associated with the quasi localized 4f electrons. Employing dynamical mean-field theory, GW and the constrained random phase approximation, we computed the actual colour (the RGB code) of a CeSF paint-coating, using only the atomic positions as inputs. We further identified a non-conventional inter-atomic transition scenario that explains CeSF's excellent pigmentation properties, showcasing the power of modern electronic structure methods that open up new possibilities of materials design.

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M. Gamza, A. Puri, JMT, J. Quinn, M. Aronson, in preparation (2013)
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