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EINLADUNG zum IFP-SEMINAR

Extreme electronic structure modifications in off-stoichiometric $Fe_{2-2x}V_{1-x}Al_{1+3x}$

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Host:	Andrej Pustogow
Termin:	Mittwoch, 29.05.2024, 16:00 Uhr
Ort:	TU Wien, Freihausgebäude Wiedner Hauptstraße 8-10, 1040 Wien Seminarraum DC rot 07 (roter Bereich, 7. OG)

Abstract:

Guided by the Slater-Pauling principle, Heusler compounds have emerged as an important class of functional materials that provide a rich playground for fundamental and applied materials research including thermoelectrics.

In this talk, I reveal an unprecedented violation of this rule and the discovery of novel full-Heusler semiconductors experimentally as well as theoretically. Employing state-of-the-art density functional theory (DFT) methods, the occurrence of non-magnetic semiconducting ground states in highly off-stoichiometric full-Heusler alloys is theoretically predicted. This unexpected and anomalous trend is confirmed for the case of $Fe_{2-2x}V_{1-x}Al_{1+3x}$ by thermoelectric transport and magnetic measurements on a multitude of samples with varying stoichiometry. These materials exhibit vanishing magnetization and the highest measured Seebeck coefficient values of any *p*-type full-Heusler systems. Moreover, experimental, and theoretical results indicate extremely flat bands arising right below the Fermi level in these compounds.

Subsequently, the low-temperature transport properties are scrutinized, revealing non-Fermi-liquid behavior in the resistivity and signatures of weak anti-localization, together with extremely low Hall mobilities.

Calculations on numerous other full-Heusler alloys, based on $X_{2-2x}Y_{1-x}Z_{1+3x}$, reveal similar (semiconducting) electronic structures. This proves the generality of this approach and motivates further studies on highly off-stoichiometric Heusler compounds with intriguing physical properties.