TECHNISCHE UNIVERSITÄT DRESDEN

Institut für Festkörper- und Materialphysik

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IFMP Seminar

Date Monday, June 10, 2024, at 14:50

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Speaker **Esteban Zuñiga-Puelles**
TU Bergakademie Freiberg

Title **Thermal and electrical transport in natural and synthetic sulfur-based semiconductors**

Abstract The pursuit for efficient and sustainable energy generation has prompted the exploration of various technologies, among which thermoelectricity-stands out as a captivating field of study with potential applications. It allows the direct conversion of thermal (heat-gradient) into electrical energy, that could be employed for power generation from waste heat in industrial processes, automotive exhaust systems, etc. The thermoelectric (TE) performance of a material is commonly evaluated by the dimensionless figure of merit, $zT = S^2T/\rho\kappa_{tot}$, (with ρ the electrical resistivity, S the Seebeck coefficient, and κ_{tot} the total thermal conductivity) and it is desired to be as high as possible (i.e., for state-of-the-art materials $zT \geq 1$).

Pyrite (FeS_2), Galena (PbS) and In-thiospinels ($In_{1-y}\bullet_y In_2S_{4-x}Te_x$) are semiconducting chalcogenides, stable under atmospheric conditions and composed of earth-abundant elements. These materials possess attractive electrical and/or thermal transport properties, making them the focus of several theoretical and experimental studies for potential thermoelectric applications. Large natural pyrite and galena crystals as well as synthetic polycrystalline $In_{1-y}In_2S_{4-x}Te_x$ and FeS_2 have been characterized by several methods and found to be of outstanding chemical and structural quality (rivaling those previously reported). Such thorough sample characterization allows us to elucidate the intrinsic properties of the respective systems, where the underlying processes governing their electrical and thermal transports have been studied.

[1] *Structural stability and thermoelectric performance of high quality synthetic and natural pyrites (FeS_2)*, Dalton Transactions **48**, 10703–10713 (2019).

[2] *Thermoelectric properties and scattering mechanisms in natural PbS*, Physical Review B **107**, 195203 (2023).

[3] *Thermoelectric performance of indium-rich thiospinels $In_{1-y}\bullet_y In_2S_{4-x}Te_x$ ($y \approx 0.16, 0.22$ and $x \approx 0.1, 0.2$)*, Journal of Alloys and Compounds **976**, 173055 (2024).

Host: D. Peets

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