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Thermopower as a probe of electronic correlations: the case of antiferromagnetic UNi_{0.34}Ge₂

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U-TE-Ge compounds exhibit remarkable coexistence of ferromagnetism and superconductivity which attracts attention of the scientific community to study unique physical properties and potential applications in nuclear industry. The orthorhombic crystal structure is characterized by layers with U atoms in zigzag chains. Recently synthesized UNi_{0.34}Ge₂ is so far the only exception in this family because it orders antiferromagnetically below 45 K and superconductivity has not been observed yet. Highly anisotropic magnetic structure with two easy axes was observed in magnetization, specific heat, thermal expansion [1] and in transport measurements.

Ab initio calculations are challenging in this case because of U-5f electrons near the Fermi level and structural disorder. Usually, strongly interacting U-5f electrons are described with DFT+U approach in which the parameters are chosen to reproduce, for example the experimentally determined magnetic moments or XPS spectrum. In this work we demonstrate that the thermopower, which is frequently much easier to be experimentally determined, is a sensitive probe of electronic correlations which may be successfully used to assess the magnitude of electronic correlations. The electronic structure and thermopower of UNi_{0.34}Ge₂ was calculated using DFT methods [2,3] and we found that Seebeck coefficient is more sensitive to the choice of Hubbard U and J parameters than e.g. magnetic moments and compared to experiment allows to properly determine their values.

References

- [1] A. Pikul et al., Phys. Rev. Materials 6, 104408 (2022).
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- [3] G. Madsen et al., Comput. Phys. Commun. 231,140-145 (2018)

Primary authors: GAGOR, A. (Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland); PIKUL, A. (Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland); WIENDLOCHA, B. (Faculty of Physics and Applied Computer Science, AGH University of Krakow, Krakow, Poland); KUDEROWICZ, G. (Faculty of Physics and Applied Computer Science, AGH University of Krakow, Poland); GOFRYK, K. (Glenn T. Seaborg Institute, Idaho National Laboratory, Idaho Falls, ID 83415, USA); REGMI, K. (Center for Quantum Actinide Science and Technology, Idaho National Laboratory, USA); OHASHI, M. (Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan); PASTUREL, M. (Univ Rennes, CNRS, Institut des Sciences Chimiques de Rennes, UMR6226, Rennes, France); SZLAWSKA, M. (Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland)

Presenter: KUDEROWICZ, G. (Faculty of Physics and Applied Computer Science, AGH University of Krakow, Poland)

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