

DISTINGUISHED LECTURE SERIES

Winter Term 2021/2022

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Functional magnetocaloric materials on atomic length scales: element specific insight

To achieve a fundamental understanding of the hysteresis of new magnetocaloric systems on atomic length scales, I will present element specific studies of these functional materials. The techniques utilized are X-ray absorption spectroscopy (XAS) and nuclear resonant inelastic X-ray scattering (NRIXS) at synchrotron radiation facilities as well as laboratory-based Mössbauer spectroscopy studies. In contrast to permanent magnets with a maximized magnetic hysteresis, magnetocaloric systems shall present a minimized (thermal) hysteresis [1,2]. The tailoring of hysteresis is a crucial task which is tackled by modifying structural phase transitions in these materials. To understand the interplay of local atomic magnetic properties with the lattice dynamics, the study of element specific thermodynamics is essential for the analysis of the coupling of lattice and magnetic degrees of freedom. This is achieved by NRIXS measurements, revealing the modification of the vibrational density of states versus temperature along the first or second order phase transition [3,4]. The experimentally determined local magnetic properties can be ideally compared to results by density functional theory. Thereby the cross-coupling between magnetic, electronic and vibrational degrees of freedom (spin-phonon coupling) is analyzed. Based on the thorough understanding of microscopic mechanisms governing the shape of the free energy surface, we aim to identify relevant strategies to tailor the interactions. Examples will be presented for the magnetocaloric materials $\text{LaFe}_{13-x}\text{Si}_x$ [3-6] and FeRh [7,8].

- [1] F. Scheibel et al., *Energy Technol.* 6 (8), 1397-1428 (2018)
- [2] O. Gutfleisch et al., *Phil. Trans. R. Soc. A* 347, 20150308 (2016)
- [3] M. E. Gruner et al., *Phys. Rev. Lett.* 114, 057202 (2015)
- [4] M. E. Gruner et al., *Phys. Status Solidi B* 255, 1700465 (2018)
- [5] A. Terwey et al., *Phys. Rev. B* 101, 064415 (2020)
- [6] J. Landers et al., *Phys. Rev. B* 98, 024417 (2018)
- [7] B. Eggert et al., *RSC Adv.* 10, 14386-14395 (2020)
- [8] M. Wolloch et al., *Phys. Rev. B* 94, 174435 (2016)

Date: **Monday, December 13, 2021**

Time: **04:00 pm**

Venue: **On site 46/HS 270 or Online via Zoom; the speaker is joined by Zoom**

Meeting ID: **641 9279 3075**, Passcode: **4Ko!!2122**, Link:

<https://uni-kl-de.zoom.us/j/64192793075?pwd=WnlJYWWh4ZENmV2tWZk12UolHRUthUT09>