

SEMINARIUM Z MAGNETYZMU I NADPRZEWODNICTWA

Uprzejmie zawiadamiamy, że w **środe**

24 marca 2021 r., o godz.10:00

odbędzie się seminarium **on-line (link podany jest na stronie IF PAN),**

na którym

dr Konrad J. Kapcia

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wyłosi referat na temat:

“Ab initio calculations of electronic structures and phonon spectra for selected noncentrosymmetric superconducting systems”

The absence of an inversion center induces the antisymmetric spin-orbit coupling, enabling a mixture of the spin-singlet and spin-triplet Cooper pairing. Here, two different superconducting systems will be discussed. For the series of noncentrosymmetric superconductors ThXSi, where $X = \text{Co, Ni, Ir, and Pt}$ [1], we performed the density functional theory studies [2]. We analyzed the effect of the spin-orbit coupling, which splits the degenerate electronic states and modifies the Fermi surfaces. The calculated phonon spectra strongly depend on atom type X , showing a tendency for dynamical instability in ThCoSi and ThIrSi. The second material is $\text{Cd}_2\text{Re}_2\text{O}_7$ compound. It is the first discovered pyrochlore oxide superconductor [3]. We studied the structural and phonon properties of the high-temperature cubic and two low-temperature tetragonal phases [4]. We revealed the soft mode in the Brillouin zone center, which breaks the tetragonal symmetry and induces the orthorhombic structure. This result explains the recent Raman measurements.

The research is partially financed by National Science Centre (NCN, Poland) under the research project SONATINA 1, grant. no. 2017/24/C/ST3/00276.

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[3] M. Hanawa, Y. Muraoka, T. Tayama, T. Sakakibara, J. Yamaura, Z. Hiroi, *Phys. Rev. Lett.* 87, 187001 (2001); H. Sakai, K. Yoshimura, H. Ohno, H. Kato, S. Kambe, R. E. Walstedt, T. D. Matsuda, Y. Haga, Y. Onuki, *J. Phys.: Condens. Matter* 13, L785 (2001).

[4] K. J. Kapcia, M. Reedyk, M. Hajialamdari, A. Ptok, P. Piekarczyk, A. Schulz, F. S. Razavi, R. K. Kremer, A. M. Oleś, *Phys. Rev. Research* 2, 033108 (2020).

Serdecznie zapraszamy

Roman Puźniak
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