# SEMINAR ON MAGNETISM AND SUPERCONDUCTIVITY

We kindly inform You that on **Wednesday**

## March 5th at 10:00

there will be a ZOOM **seminar,**

where


## Dr. Eng. Michał J. Winiarski

*(Faculty of Applied Physics and Mathematics and Advanced Materials Center, Gdansk University of Technology, ul. Narutowicza 11/12, 80-233 Gdansk, Poland)*


will deliver a lecture on:

# "Can analysis of chemical bonding help us find new superconductors?"

Superconductors hold immense importance in many fields of current technology, including power transmission, medical imaging, high-sensitivity measurements, and more recently - quantum computing. However, despite more than 110 years have passed since the discovery of superconductivity, a universally applicable set of rules for designing superconducting materials remains elusive.

Recently a correlation between the occurrence of superconductivity and the presence of antibonding states at the Fermi level was found in several groups of materials (see eg. [1-3]). The phenomenon can be qualitatively understood as an unusual form of bonding optimization – relieving the electronic "stress" due to occupied antibonding states via an electronic structure "distortion". Such a concept was previously proposed to rationalize the occurrence of itinerant ferromagnetism in intermetallic compounds [4].

I will present the results of chemical bonding analysis employing the molecular orbital theory and DFT-based bonding descriptors (eg. crystal orbital Hamilton population function – COHP) on several superconducting Heusler phases and endohedral cluster compounds [5,6]. I would also like to discuss the possibility of employing these methods to highlight new superconductor candidates.


*[1] S. Gutowska et al., J. Phys. Chem. C.* ***127*** *(2023) 14402-14414*
*[2] X. Gui et al., Chem. Mater.* ***30*** *(2018) 6005-6013*
*[3] V.Y. Verchenko, A.A. Tsirlin, A.V. Shevelkov, Inorg. Chem. Front.* ***8*** *(2021) 1702-1709*
*[4] G.A. Landrum, R. Dronskowski, Angew. Chem. Int. Ed.* ***39*** *(2000) 1560-1585*
*[5] Z. Ryżyńska et al., Chem. Mater.* ***32*** *(2020) 3805-3812*
*[6] Z. Ryżyńska et al., J. Phys. Chem. C.* ***125*** *(2021) 11294-11299*


**The lecture will be in Polish, the slides will be in English.**

**We sincerely invite You**

**Roman Puźniak / Andrzej Szewczyk / Henryk Szymczak**