**Structure–property relationships in Fe–Ge intermetallics:
Spotlight on Nowotny Chimney Ladders**

**I. Lukashchuk1, O. Cherniushok1, T. Parashchuk1, K. Pryga2, B. Wiendlocha2, J. Toboła2, A. Zevalkink3, Y. Grin4, K. T. Wojciechowski1**

### 1AGH University of Krakow, Faculty of Materials Science and Ceramics, Department of Inorganic Chemistry, Thermoelectric Research Laboratory, Mickiewicza Ave. 30, 30-059 Krakow, Poland

###  2Faculty of Physics and Applied Computer Science, AGH University of Krakow, 30-059 Krakow, Poland

### 3Michigan State University, East Lansing, USA

### 4Max Planck Institute of Chemical Physics of Solids, Dresden, Germany

*iluka@agh.edu.pl*

The crystal structure of a material fundamentally dictates its electronic and thermal transport properties, making it a critical factor in determining thermoelectric performance [1]. This research explores this profound influence by focusing on three distinct FeGe, Fe2Ge3, and FeGe2 phases in the Fe-Ge system [2]. Despite being built from iron and germanium atoms, these compounds exhibit unique stoichiometric ratios and, crucially, possess vastly different crystal structures. This structural diversity is hypothesized to significantly alter their electronic band structures and phonon scattering mechanisms, which are fundamental to efficient thermoelectric energy conversion.

A particular emphasis is placed on the Nowotny Chimney Ladder (NCL) Fe2Ge3 phase. The obtained results reveal that NCL Fe2Ge3 exhibits a significantly enhanced Seebeck coefficient of up to -165.4 µVK-1 compared to approximately 10 µVK-1 for FeGe and
-3 µVK-1 for FeGe2, leading to a higher power factor of 14.3 µWcm-1K-2. Furthermore, its unique crystal structure contributes to remarkably lower lattice thermal conductivity 1.6 Wm-1K-1 at room temperature relative to its counterparts (FeGe 2.9 Wm-1K-1 and FeGe2 around 4.2 Wm-1K-1). This combination of enhanced electronic and disturbed thermal transport results in NCL Fe2Ge3 demonstrate the highest thermoelectric figure of merit (*ZT*) among all three phases at relevant temperatures, achieving a peak *ZT* of 0.43 at 623 K. By meticulously correlating the individual crystal structure of FeGe, NCL Fe2Ge3, and FeGe2 with their measured and calculated transport parameters, we demonstrate that crystal structure profoundly impacts charge carrier dynamics and phonon scattering. Our results confirm that crystal structure engineering is a powerful strategy for optimizing high-performance thermoelectric materials, with NCL Fe2Ge3 serving as a compelling example for future material design.

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[2] S. Tonquesse, C. Hassam, Y. Michiue, Y. Matsushita, M. Pasturel, T. Mori, T. S. Suzuki, D. *Journal of Alloys and Compounds*. 2020, 846, 155696.

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