Recent Advances in Thermoelectric properties of MXenes-based nanomaterials and beyond

Magdalena Birowska^{1,} Subrahmanyam Bandaru¹, Agnieszka M. Jastrzębska²

¹Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland, subrahmanyam.bandaru@fuw.edu.pl

²University of Technology, Faculty of Materials Science and Engineering, 02-507 Warsaw, Wołoska 141, Poland

Energy plays a key role in the development of civilization. Yet, the energy production is still dominated by non-renewable fossil fuels. In the search of novel and sustainable forms of energy, thermoelectric (TE) materials attract the enormous attention because they assist in recovering the energy from wasted heat. However, the efficiency of the existing TE materials operating in room temperature is still not satisfactory. Recently, MXenes a two-dimensional (2D) materials, gained a significant attention since theirs atomically thin layers exhibit unique band structures that enable to attain large thermoelectric power factors [1].

In this review, I will briefly discussed various aspects and the importance of thermoelectrics materials (TM). I will focus on thermoelectric properties of MXenes in comparison to conventional TM and other 2D materials [2]. I will present various strategies in enhancing the thermoelectric figure of merit (ZT), Seebeck coefficient, and termoelectric power of MXenes-based nanomaterials. In particular, the defective surfaces play a key role in reducing the thermal conductivity of MXenes. Moreover, the range of MXenes chemical composition enables the research path via energy band engineering, optimization, carrier concentration and mobility. Additionally, the latest addition to the flatland, transition metal borides (MBenes) demonstrates an incredible diversity of structures with various crystal symmetries [3,4]. Finally, other aspects such as layer-dependent TE properties and structural anisotropy, which lead to the orientation dependent properties, pave the way in device design for potential TE applications. The commercial applications of TE devices will be also partially discussed, with possibilities and prospects extended to MBenes.

[1] S. Karmakar and T. Saha-Dasgupta, *First-principles prediction of enhanced thermoelectric properties of double transition metal MXenes:* $Ti_{3-x}Mo_xC_2T_2$; (x=0.5,1,1.5,2,2.5,T=-OH/-O/-F), Phys. Rev. Mat. **4**, 124007 (2020).

[2] S. Bandaru, A. M. Jastrzębska M. Birowska, *Recent progress in thermoelectric MXene-based structures versus other 2D materials*, https://arxiv.org/abs/2304.07015.

[3] V. G. Nair, M. Birowska, D. Bury, M. Jakubczak, A. Rosenkranz, and A. M. Jastrzębska, 2D MBenes: A Novel Member in the Flatland, Advanced Materials 34, **4** 2108840 (2022),

[4] M. Jakubczak, A. Szuplewska, A. Rozmysłowska-Wojciechowska, A. Rosenkranz, and A. M. Jastrzębska, *Novel 2D MBenes - Synthesis, Structure, and Biotechnological Potential*, Advanced Functional Materials **31**, 2103048 (2021)