Guangzong Xing
Ningbo Institute of Materials Technology and Engineering (NIMTE)
1219 West Zhongguan Road, Zhenhai District, Ningbo, 315201, CHINA
xingguangzong@nimte.ac.cn

EDUCATION

September 2015-December 2018: Doctor's degree from College of Materials Science and Engineering, Jilin University

Major:	Materials Physics and Chemistry
Advisor:	Dr. Weitao Zheng (Jilin University)
Co-Advisor:	Dr. David J. Singh (University of Missouri-Columbia)
Co-Advisor:	Dr. Xiaofeng Fan (Jilin University)
Research Fields:	Exploring new functional materials (thermoelectric materials, phase change memory materials, and magnetic materials) using first-principles calculations based on DFT.

September 2013-June 2015: Master's courses from College of Materials Science and Engineering, Jilin University.
Major: Materials Physics and Chemistry (*Ranked first in the major*)

September 2009-June 2013: Bachelor's degree from College of Materials Science and Engineering, Jilin University.
Major: Materials Physics (*Graduated among top 10% of the class*)

RESEARCH EXPERIENCE

June 2024-prsent: Associate professor at Ningbo Institute of Materials Technology and Engineering (NIMTE)

- Develop computational programs for designing thermoelectric and magnetic materials based on density functional theory (DFT) first-principles calculations.
- Assist in the development of new materials through high-throughput computing and machine learning.

April 2020-May 2024: Postdoctoral Fellow at National Institute for Materials Science (NIMS)

- Lattice dynamics effects on phase stability and magnetocrystalline anisotropy energy (MAE) of $R_{1-x}(Fe,Co)_x$ compounds at finite temperature.
- Prediction of new magnetic and spintronic materials using first-principles calculations and machine learning techniques.

March 2019-March 2020: Postdoctoral Fellow at Okinawa Institute of Science and Technology Graduate University (OIST)

- Investigated the transport properties of organic systems with phonon-electron interaction based on Molecular Dynamics.

September 2016-September 2018: Visiting scholar at the University of Missouri-

Columbia

- Constructed an electronic fitness function for screening semiconductors as thermoelectric materials based on Boltzmann transport theory.
- Predicted the crystal structure of the phase change memory material Sn_2Se_3 and investigated its electronic properties.
- Investigated the thermoelectric properties of cubic and rhombohedral GeTe.

PUBLICATIONS

G. Xing*, K. Masuda, T. Tadano, Y. Miura, "Chemical-substitution-driven giant anomalous Hall and Nernst effects in magnetic cubic Heusler compounds", *Acta Mater.*, 270, 119856 (2024).

G. Xing*, Y. Miura, and T. Tadano, "First-principles prediction of phase transition of YCo_5 from self-consistent phonon calculations", *Phys. Rev. B* 108, 014304 (2023).

G. Xing*, Y. Miura, and T. Tadano, "Lattice dynamics and its effects on magnetocrystalline anisotropy energy of pristine and hole-doped YCo_5 from first principles", *Phys. Rev. B* 105, 104427 (2022).

G. Xing*, T. Ishikawa, Y. Miura, T. Miyake, T. Tadano, "Lattice dynamics effects on finite-temperature stability of $R_{1-x}Fe_x$ (R = Y, Ce, Nd, Sm, and Dy) alloys from first principles" *J. Alloys Compd.* 874, 159754 (2021).

G. Xing, Y. Li, Z. Feng, D. J. Singh, and F. Pauly, "Copper(I)-Based Flexible Organic-Inorganic Coordination Polymer and Analogues: High-Power Factor Thermoelectrics" *ACS Appl. Mater. Interfaces* 12, 53841 (2020).

G. Xing, L. Shang, Y. Fu, W. Ren, X. Fan, W. Zheng, D. J. Singh, "Structural instability and magnetism of superconducting KCr_3As_3" *Phys. Rev. B* 99, 174508 (2019).

G. Xing, J. Sun, Y. Li, X. Fan, W. Zheng, D. J. Singh, "Thermoelectric Properties of p-type Cubic and Rhombohedral GeTe" *J. Appl. Phys.* 123, 195105 (2018).

G. Xing, J. Sun, Y. Li, X. Fan, W. Zheng, D. J. Singh, "Electronic fitness function for screening semiconductors as thermoelectric materials" *Phys. Rev. Mater.* 1, 065405 (2017).

G. Xing, Y. Li, X. Fan, L. Zhang, W. Zheng, and D. J. Singh, "Sn_2Se_3: A conducting crystalline mixed valent phase change memory compound" *J. Appl. Phys.* 121, 225106 (2017).

G. Xing, J. Sun, K. P. Ong, X. Fan, W. Zheng, and D. J. Singh, "Perspective: n-type oxide thermoelectrics via visual search strategies" *APL Mater.* 4, 053201 (2016).

G. Xing, X. Fan, W. Zheng, Y. Ma, H. Shi, and D. J. Singh, "Magnetism in Na-filled Fe-based skutterudites" *Sci. Rep.* 5, 10782 (2015).

I. Kurniawan, Y. Miura, **G. Xing**, T. Tadano, K. Hono, "Theoretical study of the effect of lattice dynamics on the damping constant of FePt at finite temperature" *Phys. Rev. B* 108, 094426 (2023)

Z. Ren, S. Tian, J. Noh, F. Oviedo, **G. Xing**, J. Li, Q. Liang, R. Zhu, A. Aberle, S. Sun, X. Wang, Y. Liu, Q. Li, S. Jayavelu, K. Hippalgaonkar, Y. Jung, and T. Buonassisi, "An invertible crystallographic representation for general inverse design of inorganic crystals with targeted properties" *Matter* 5, 314 (2021).

T. Ishikawa, T. Fukazawa, **G. Xing**, T. Tadano, T. Miyake, "Evolutionary search for cobalt-rich compounds in the yttrium-cobalt-boron system" *Phys. Rev. Mater.* 5,054408 (2021).
H.H Huang, **G. Xing**, X. Fan, D. J. Singh, W. Zheng, "Layered Tl_2O: a model thermoelectric material" *J. Mater. Chem. C* 7, 5094 (2019).
K. M. Taddei, **G. Xing,** J. Sun, Y. Fu, Y. Li, Q. Zheng, A. S. Sefat, D. J. Singh, C. de la. Cruz, "Frustrated structural instability in superconducting quasi-one-dimensional $K_2Cr_3As_3$" *Phys. Rev. Lett.* 121,187002 (2018).
A. Putatunda, **G. Xing**, J. Sun, Y. Li, D. J. Singh, "Thermoelectric properties of layered $NaSbSe_2$" *J. Phys.: Condens. Matter.* 30, 225501 (2018).
J. P. Sun, P. Shahi, X. Zhou, Y. L. Huang, K. Y. Chen, B. S. Wang, S. L. Ni, N. N. Li, K. Zhang, W. G. Yang, Y. Uwatoko, **G. Xing**, J. Sun, D. J. Singh, K. Jin, F. Zhou, G. M. Zhang, X. L. Dong, Z. X. Zhao, and J.-G. Chen, "Reemergence of high-T_c superconductivity in the $(Li_{1-x}Fe_x)OHFe_{1-y}Se$ under high pressure" *Nat. Commun*. 9, 380 (2018).

(*: corresponding author)

EXPERTISE

- Extensive experience in first-principles calculations using VASP and WIEN2k.
- Crystal structure prediction using CALYPSO.
- Boltzmann transport calculations using BoltzTraP.
- Anharmonic phonon calculations using ALAMODE code

CONFERENCE PRESENTATIONS

The 2023 JSAP Autumn Meeting Sep 19-23, 2023 Kumamoto Japan

- "High-throughput Calculation of Transverse Transport Properties in Doped Heusler Compounds" (oral presentation)

The 2023 Intermag Meeting May 15-19, 2023 Sendai Japan

- "High-throughput Calculation of Transverse Transport Properties in Heusler Compounds " (poster presentation)

The 2022 American Physical Society March Meeting March 14-18, 2022 online meeting

- "Lattice dynamics effects on magnetocrystalline anisotropy energy of YCo_5 from first principles" (oral presentation)

The 2021 American Physical Society March Meeting March 15-19, 2021 online meeting

- "$R_{1-x}Fe_x$ (R = Y, Ce, Nd, Sm, and Ce) compounds: Temperature-induced phase stabilization effect at finite temperature" (oral presentation)

Hands-on DFT and beyond workshop Aug 26-Sep 6, 2019 Barcelona Spain

- "Structural instability and magnetism of superconducting KCr_3As_3" (poster presentation)

The 2018 American Physical Society March Meeting Mar 05-09, 2018 Los Angeles USA

- "Screening for Potential Thermoelectric Materials using an Electronic Fitness Function" (oral presentation)

The 2017 American Physical Society March Meeting Mar 13-17, 2017 New Orleans USA

- "Structure and Electronic Properties of mixed-valence compound Sn_2Se_3" (oral presentation)

2nd Doctoral Forum in Physics Dec 17-19, 2014 Beijing China

- "Magnetism in Na-filled Fe-based skutterudites" (oral presentation)

AWARDS

2009-2013	Full University Scholarship
2013-2015	Postgraduate Students Basic Scholarship
	Postgraduate Students Excellence Scholarship
2015-2018	Postgraduate Students Basic Scholarship
	Postgraduate Students Excellence Scholarship