

YUELEI BAI

Associate Professor

Centre for Composite Materials and Structures,
Harbin Institute of Technology

Room 420, A building, 2# Yikuang Street, Harbin 150080

Email: baiyl@hit.edu.cn; baiyl.hit@gmail.com

Homepage: homepage.hit.edu.cn/baiyuelei

ReseracherID: www.researcherid.com/rid/B-1510-2010

Google scholar: scholar.google.com.sg/citations?user=d21mW3YAAAAJ&hl=zh-CN



RESEARCH AREA & INTERESTS

Computational materials science: Theoretical design and prediction of ternary transition-metal layered phases using First-principle

Ceramic materials science: Synthesis and characterization of ternary transition-metal layered phases

Solid mechanics: Fracture and damage of quasi-brittle materials (MAX phases)

EDUCATION

Harbin Institute of Technology, Harbin, China

PhD student in Engineering Mechanics (Sep 2006-June 2012)

PhD project: Characterization for properties of bulk Ti_2AlC synthesized by combustion synthesis and First-principle study on MAX phases

Harbin Institute of Technology, Harbin, China

Undergraduate in Composite Material and Engineering (Sep 2002-July 2006), with Distinction

Degree of B. Eng: Preparation and Property of Aluminum Electrolysis Inert Alloy Anode Material (2006)

RESEARCH EXPERIENCE

Center for Composite Materials and Structures, Harbin Institute of Technology, Harbin, China

Associate Professor (Jan 2014 – present)

Center for Composite Materials and Structures, Harbin Institute of Technology, Harbin, China

Lecturer (July 2012 – Dec 2013)

School of Mechanical & Aerospace Engineering, Nanyang Technological

University, Singapore

Research Fellow (April 2015 – Mar 2016)

Supervisor: Dr. Kun Zhou

Research area: First-principle study on two-dimension transition carbides MXenes

Department of Materials, Imperial College London, London, UK

Sponsored Researcher (Feb 2014 – Jan 2015)

Supervisor: Prof. William E Lee and Prof. M. W. Finnis

Research area: Modelling and phase equilibria in MAX phases

Material Science Centre, University of Manchester, Manchester, UK

Visiting Student (July – Sep. 2011)

Supervisor: Prof. Ping Xiao

Research area: Microstructure characterization of Ti₂AlC (TEM)

Center for Composite Materials and Structures, Harbin Institute of Technology, Harbin, China

PhD thesis (Sep 2006 – Jun 2012)

Supervisor: Prof. Xiaodong He

Research areas: MAX phases, Ti₂AlC, Ab initio calculation, Combustion Synthesis

Center for Composite Materials and Structures, Harbin Institute of Technology, Harbin, China

University training period (Oct 2005 – July 2006)

Supervisor: Prof. Xiaodong He

Research areas: Oxidation, Inert Alloy Anode

AWARDS AND SCHOLARSHIPS

First-class Science and Technology Awards (Natural science) of Heilongjiang province, awarded by the government of Heilongjiang province (2019)

Second-class Science and Technology Awards (Natural science) of Heilongjiang province, awarded by the government of Heilongjiang province (2015)

Selected by Marquis Who's Who in **Who's Who in the World® 2015** (32nd Edition) (2014)

Outstanding young associate professor in Harbin Institute of Technology (2013), awarded by Harbin Institute of Technology

International Postdoctoral Exchange Fellowship (2013), awarded by China Postdoctoral Council (China Government), with a RMB 300,000 grant for the research project on the “*Modelling and phase equilibria in MAX phases*” (20130004)

Third-class Academic Achievement Award of Science and Technology in Harbin (2012), awarded by Harbin

The Fifth Postgraduate “Top Student from Ten Aspects” (2012), awarded by Harbin Institute of Technology

Excellent Graduate Student (2012), awarded by Heilongjiang province

Outstanding Peer Reviewer (2011), awarded by Elsevier

CASIC Scholarship (2011), awarded by China Aerospace Science & Industry Corp

Excellent PhD thesis in process (2010), awarded by Harbin Institute of Technology

CNPC Scholarship (2010), awarded by China National Petroleum Corporation

Excellent paper in Forum for PhD Students (2010), awarded by School of Aeronautics, Harbin Institute of Technology

Excellent Thesis for the Degree of B. Eng. (2006), awarded by Harbin Institute of Technology

Third-class People’s Scholarship (2002–2005), awarded by Harbin Institute of Technology

PUBLICATIONS

Issued Patents

1. Xiaodong He, **Yuelel Bai**, and Chuncheng Zhu, A Method of preparing Nb₄AlC₃ ceramic powders, **China Patent , No: 200910073098.2**
2. Xiaodong He, **Yuelel Bai**, and Chuncheng Zhu, Method of preparing Nb₄AlC₃ bulk ceramics, **China Patent , No: 200910073097.8**
3. Xiaodong He, **Yuelel Bai**, and Chuncheng Zhu, Method of preparing Nb₂AlC bulk ceramics, **China Patent , No: 200910073096.3**
4. Xiaodong He, Chuncheng Zhu, and **Yuelel Bai**, Method for preparing high purity, compact Ti₃SiC₂ block material, **China Patent , No: 200710144802.X**
5. Xiaodong He, Chuncheng Zhu, and **Yuelel Bai**, Method of preparing high purity Ti₂AlC block material, **China Patent , No: 200710144799.1**
6. Xiaodong He, Chuncheng Zhu, and **Yuelel Bai**, Method of preparing high purity Ti₂AlC block material, **China Patent , No: 200710144801.5**

Publications in international refereed journals

1. **Yuelel Bai**, Narasimalu Srikanth, Chee Kai Chua, Kun Zhou*. Density functional theory study of $M_{n+1}AX_n$ phases: A review. **Critical Reviews in Solid State and Material Sciences** 44(1), 56-107 (2019).
2. **Yuelel Bai***, Xinxin Qi, Xiaodong He, Dongdong Sun, Fanyu Kong, Yongting Zheng, Rongguo Wang, Andrew Ian Duff. Phase stability and weak metallic bonding within ternary-layered borides $CrAlB$, Cr_2AlB_2 , Cr_3AlB_4 , and Cr_4AlB_6 . **J. Am. Ceram. Soc.** 102(6), 3715-3727 (2019).
3. **Yuelel Bai***, Dongdong Sun, Ning Li, Fanyu Kong, Xinxin. Qi, Xiaodong He, Rongguo Wang, Yongting Zheng. High-temperature mechanical properties and thermal shock behavior of ternary-layered MAB phases Fe_2AlB_2 . **Int. J. Refract. Met. Hard Mat.** 80, 151-160 (2019).
4. Fanyu Kong, Xiaodong He*, Qianqian Liu, Xinxin Qi, Dongdong Sun, Yongting Zheng, Rongguo Wang, **Yuelel Bai***. Enhanced reversible Li-ion storage in $Si@Ti_3C_2$ MXene nanocomposite. **Electrochemistry Communications** 97, 16-21 (2018).
5. Fanyu Kong, Xiaodong He*, Qianqian Liu, Xinxin Qi, Dongdong Sun, Yongting Zheng, Rongguo Wang, **Yuelel Bai***. Further surface modification by carbon coating for in-situ growth of Fe_3O_4 nanoparticles on MXene Ti_3C_2 multilayers for advanced Li-ion storage. **Electrochimica Acta** 289, 228-237 (2018).
6. Fanyu Kong, Xiaodong He, Qianqian Liu, Xinxin Qi, Yongting Zheng, Rongguo Wang, **Yuelel Bai***. Effect of Ti_3AlC_2 precursor on the electrochemical properties of the resulting MXene Ti_3C_2 for Li-ion batteries. **Ceramics International** 44 [10], 11591-11596 (2018).
7. Fanyu Kong, Xiaodong He*, Qianqian Liu, Xinxin Qi, Yongting Zheng, Rongguo Wang, **Yuelel Bai***. Improving the electrochemical properties of MXene Ti_3C_2 multilayer for Li-ion batteries by vacuum calcination. **Electrochimica Acta** 265, 140-150 (2018).
8. Ning Li, **Yuelel Bai***, Shuai Wang, Yongting Zheng, Fanyu Kong, Xinxin Qi, Rongguo Wang, Xiaodong He, Andrew Ian Duff. Rapid synthesis, electrical and mechanical properties of polycrystalline Fe_2AlB_2 bulk from elemental powders. **J. Am. Ceram. Soc.** 100 [10], 4407-4411 (2017).
9. **Yuelel Bai***, Fanyu Kong, Xiaodong He, Ning Li, Xinxin Qi, Yongting Zheng, Chuncheng Zhu, Rongguo Wang and Andrew Ian Duff. Thermal shock behavior of Ti_2AlC from 200 °C to 1400 °C. **J. Am. Ceram. Soc.** 100 [9], 4190-4198 (2017).
10. **Yuelel Bai***, Xinxin Qi, Andrew Duff, Ning Li, Fanyu Kong, Xiaodong He, Rongguo Wang and Willam Edward Lee. Density functional theory insights into ternary layered boride $MoAlB$. **Acta Mater.** 132, 69-81 (2017).

11. Fanyu Kong, Ke Feng, **Yuelel Bai***, Ning Li, Xinxin Qi, Yongting Zheng, Rongguo Wang, Xiaodong He. Oxidation behavior of high-purity nonstoichiometric Ti_2AlC powders in flowing air. **J. Mater. Res.**, **32**, 2747-2754 (2017).
12. **Yuelel Bai***, Andrew Duff, Daniel Doni Jayaseelan, Rongguo Wang, Xiaodong He, and William Edward Lee. DFT Predictions of Crystal Structure, Electronic Structure, Compressibility, and Elastic Properties of Hf–Al–C Carbides. **J. Am. Ceram. Soc.** 99[10], (2016) 3449-3457.
13. **Yuelel Bai**, Kun Zhou*, Narasimalu Srikanth, John H. L. Pang, a Xiaodong He and Rongguo Wang. Dependence of elastic and optical properties on surface terminated groups in two-dimensional MXene monolayers: a first-principles study. **Rsc Advances** 6[42], (2016) 35731-39.
14. **Yuelel Bai***, Xiaodong He* and Rongguo Wang. Lattice dynamics of Al-containing MAX-phase carbides: a first-principle study. **J. Raman Spectrosc.** 46[9], (2015) 784-94.
15. **Yuelel Bai***, Xiaodong He*, Rongguo Wang, Shuai Wang, and Fanyu Kong. Effect of transition metal (M) and M-C slabs on equilibrium properties of Al-containing MAX carbides: an *ab initio* study. **Comp. Mater. Sci.** 91, (2014) 28-37.
16. **Yuelel Bai***, Huixing Zhang, Xiaodong He*, Chuncheng Zhu, Rongguo Wang, Yue Sun, Guiqing Chen, Ping Xiao. Growth morphology and microstructural characterization of nonstoichiometric Ti_2AlC bulk synthesized by self-propagating high temperature combustion synthesis with pseudo hot isostatic pressing. **Int. J. Refract Met. H.** 45, 58-63 (2014).
17. **Yuelel Bai***, Xiaodong He*, Rongguo Wang, Chuncheng Zhu. An *ab initio* study on compressibility of Al-containing MAX phases carbides. **J. Appl. Phys.** **114**, 173709 (2013).
18. **Yuelel Bai***, Xiaodong He*, Rongguo Wang, Yue Sun, Chuncheng Zhu, Shuai Wang, Guiqing Chen. High temperature physical and mechanical properties of large-scale Ti_2AlC bulk synthesized by self-propagating high temperature combustion synthesis with pseudo hot isostatic pressing. **J. Eur. Ceram. Soc.** **33**, 2435-2445 (2013).
19. **Yuelel Bai**, Xiaodong He*, Chuncheng Zhu, Guiqing Chen. Microstructures, electrical, thermal and mechanical properties of bulk Ti_2AlC synthesized by self-propagating high temperature combustion synthesis with pseudo hot isostatic pressing. **J. Am. Ceram. Soc.** **95**[1], (2012) 358-364.
20. Xiaodong He*, **Yuelel Bai**, Chuncheng Zhu, M. W. Barsoum. Polymorphism of

newly-discovered Ti_4GaC_3 : A first-principle study. **Acta Mater.** **59**, (2011) 5523-5533.

21. Xiaodong He*, **Yuelel Bai**, Yang Chen, Chuncheng Zhu, Mingwei Li. Phase stability, electronic structure, compressibility, elastic and optical properties of a newly discovered Ti_3SnC_2 : A First-principle study. **J. Am. Ceram. Soc.** **94**[11], 3907-3914 (2011).
22. Xiaodong He*, **Yuelel Bai**, Chuncheng Zhu, Yue Sun, Mingwei Li, and M. W. Barsoum. General trends in the structural, electronic and elastic properties of the M_3AlC_2 phases (M = transition metal): A first-principle study. **Comp. Mater. Sci.** **49**, (2010) 691-698.
23. Xiaodong He*, **Yuelel Bai**, Yibin Li, Chuncheng Zhu and Xianghao Kong. *In situ* synthesis and mechanical properties of bulk Ti_3SiC_2/TiC composites by SHS/PHIP. **Mater. Sci. Eng. A** **527**, (2010) 4554-4559.
24. **Yuelel Bai**, Xiaodong He*, Mingwei Li, Yue Sun, Chuncheng Zhu, Yibin Li. *Ab initio* study of the bonding and elastic properties of Ti_2CdC . **Solid State Sci.** **12**, (2010) 152-155.
25. **Yuelel Bai**, Xiaodong He*, Yue Sun, Chuncheng Zhu, Mingwei Li and Liping Shi. Chemical bonding and elastic properties of Ti_3AC_2 phases (A = Si, Ge, and Sn): A First-principle study. **Solid State Sci.** **12**, (2010) 1209-1214.
26. Zuo Chun-Ying*, Wen Jing, and **Bai Yue-Lei**. First-principles investigation of N Ag co-doping effect on electronic properties in p-type ZnO. **Chin. Phys. B** **19** [4], (2010) 047101.
27. **Yuelel Bai**, Xiaodong He*, Yibin Li, Chuncheng Zhu, Sam Zhang. Rapid synthesis of bulk Ti_2AlC by self-propagating high temperature combustion synthesis with pseudo hot isostatic pressing process. **J. Mater. Res.** **24**, (2009) 2528-2535.
28. Xiaodong He*, **Yuelel Bai**, Yibin Li, Chuncheng Zhu, Mingwei Li. *Ab initio* calculations for properties of MAX phases Ti_2InC , Zr_2InC , and Hf_2InC . **Solid State Commun.** **149**, (2009) 564-566.
29. **Yuelel Bai**, Xiaodong He*, Yibin Li, Chuncheng Zhu, Mingwei Li. An *ab initio* study of the electronic structure and elastic properties of the newly discovered ternary carbide Ti_4GaC_3 . **Solid State Commun.** **149**, (2009) 2156-2159.

Publication in national journals

30. Xinxin Qi, Guangping Song¹, Weilong Yin, Mingfu Wang, Xiaodong He, Yongting Zheng, Rongguo Wang, **Yuelel Bai***. Analysis on Phase Stability and Mechanical

Properties of Newly-Discovered Ternary Layered Boride Cr₄AlB₄. *Journal of Inorganic Materials* 35(1), (2020). (in Chinese)

31. Zhu Jia, Lin Hong, Zhu Chuncheng*, **Bai Yuele**i. First Principles Study of Thermodynamic Properties of Ti₂AlC. *Rare Met. Mater. Eng.* **42**, 290-292 (2013).
32. **Bai Yuele**i*, He Xiaodong, Zhu Chuncheng. The research on the oxidation behavior of Fe-Ni-Al alloy at 900 °C. *J. Harbin Institute of Technology* **40** [1], 65-68 (2008).
33. Li Chong, He Xiaodong, Zhu Chuncheng, **Bai Yuele**i. High Temperature Oxidation Behavior of Ternary Layered Ti₃SiC₂ Ceramic. *J. Eng. Mater.* **S1**, 168-171 (2006).

Impact of research outcomes

More than **576** total citations (SCI), with the H-Index of **15** (Web of Science).

CONFERENCE TALK

1. **(Keynote)** Damage-tolerant ternary layered borides MAB phases: theoretical and experimental insights. 10th International Conference on High Temperature Ceramic Matrix Composites (HT-CMC10), *Bordeaux, France* (2019).
2. **(Invited)** Ternary-layered borides MAB phases: a class of damage-tolerant ceramics. The 13th Pacific Rim Conference of Ceramic Societies (PACRIM13), *Okinawa, Japan* (2019).
3. **(Invited)** Weak bonding within the ternary layered ceramics: Origin of unusual mechanical properties. 11th International Conference on High-Performance Ceramics (CICC-11), *Kunming, China* (2019).
4. **(Invited)** Damage-tolerant ternary layered ceramics: from the MAX to MAB phases. 2019 EMN Meeting on Ceramics, *Jeju Island, Korea* (2019).
5. **(Invited)** Model of “Bond stiffness” and its role in understanding and predicting ternary-layered MAX and MAB phases. 12th International Conference on Ceramic Materials and Components for Energy and Environmental Applications 2018 (CMCEE 2018), *Singapore, Singapore* (2018).
6. **(Invited)** Unusual mechanical properties of ternary layered ceramics with high fracture toughness: Model of “Bond stiffness” and its application. 20th Annual Conference of Chinese High-performance Ceramics, *Huhot, China* (2018, in Chinese).
7. (Oral) Establishment of “Bond stiffness” model and its application in understanding the unusual mechanical properties of ternary layered ceramics. Symposium on materials mechanical behavior in special environment between USTC and HIT, *Hefei, China* (2018, in Chinese).

8. **(Invited)** Ternary layered compounds: bridge between ceramics and metal. 2nd Youth Science and Technology Forum of China Nonferrous Metals Society, *Changchun, China* (2018, in Chinese)
9. **(Invited)** New class of ternary layered borides MAB phases: Theoretical prediction, synthesis and characterization. 9th Symposium on structure, properties and characterization of inorganic materials, *Enshi, China* (2018, in Chinese).
10. **(Invited)** Theoretical insights and predictions of ternary layered boride MoAlB using first-principles. 10th International Conference on High-Performance Ceramics (CICC-10), *Nanchang, China* (2017).
11. (Oral) Density functional theory predictions of ternary layered boride MoAlB. The Chinese Congress of Theoretical and Applied Mechanics – 2017, *Beijing, China* (2017, in Chinese).
12. **(Invited)** Density functional theory insights into ternary layered boride MoAlB. 12th Pacific Rim Conference on Ceramic and Glass Technology, *Waikoloa, Hawaii, USA* (2017).
13. (Oral) Characterization of Ti₂AlC bulk synthesized by self-propagating high temperature combustion synthesis with pseudo hot isostatic pressing. 19th Annual Conference of Chinese High-performance Ceramics, *Wuhan, China* (2016, in Chinese).
14. (Oral) Synthesis and Characterization of Ti₂AlC bulk by self-propagating high temperature combustion synthesis with pseudo hot isostatic pressing. Second Sino-Russia Workshop on self-propagating high temperature combustion synthesis (SHS), *Beijing, China* (2012).
15. (Poster) Preparation of ternary layered Ti₃SiC₂ ceramic by SHS/PHIP. 5th China International Conference on High-Performance Ceramics (CICC-5), *Changsha, China* (2007).

STUDENTS SUPERVISED

Currently supervised Ph.D students:

2019 – Present Bingbing Hao

2018 – Present Xinxin Qi, with Dr. Weilong Yin

2015 – Present Fanyu Kong, with Prof. Xiaodong He

Graduated M.Phil students:

2018 – Present Jin Gao

2017 – 2019 Dongdong Sun

2016 – 2018 Xinxin Qi

2015 – 2017 Ning Li
2014 – 2016 Zheng Liang
2013 – 2014 Fanyu Kong, with Prof. Xiaodong He
2012 – 2013 Shuai Wang, with Prof. Xiaodong He

Currently supervised M.Phil students:

2017 – Present Jin Gao
2016 – Present Dongdong Sun

Previously supervised undergraduate students:

2018 Tianyu Wang, Chengyu Tao
2016 Ke Feng
2013 Fanyu Kong, with Prof. Xiaodong He

RESEAR GRANTS

Sponsor: National Natural Science Foundation of China (Grant No. 51972080)

Title: High-throughput global screening and experimental verification of high-toughness and damage-tolerant ternary-layered borides

Amount granted: RMB 600,000

Period: Jan 2020 - Dec 2023

Sponsor: National Natural Science Foundation of China (Grant No. 11302061)

Title: Theoretical Design using First-principle Calculations and Experimental Verification of New Ternary Machinable Ceramics

Amount granted: RMB 250,000

Period: Jan 2014 - Dec 2016

Sponsor: China Postdoctoral Science Foundation (Grant No. 2017T100230)

Title: Interfacial design and experimental verification of a new multi-scale reinforcement by chemically grafting two-dimension transition metal carbides MXenes onto carbon fiber

Amount granted: RMB 150,000

Period: June 2017 - Jun 2019

Sponsor: China Postdoctoral Science Foundation (Grant No. 2013M531033)

Title: First-principle study on phase stability of ternary layered machinable ceramics, and theoretical prediction of new materials

Amount granted: RMB 50,000

Period: Sep 2012 - Sep 2014

Sponsor: Research Fund for the Doctoral Program of Higher Education of China (Grant No. 20132302120024)

Title: Study on fracture and damage behavior in ternary machinable ceramics MAX

phases (Ti₂AlC)

Amount granted: RMB 40,000

Period: Jan 2014 - Dec 2016

SERVICE TO THE PROFESSION

Member: American ceramic society (lifetime), Chinese Society of Theoretical and Applied Mechanics

Referee for National Natural Science Foundation of China

Referee for international journals

Journal of American Ceramic Society, Journal of Applied Physics, Journal of the European Ceramic Society, Electrochimica Acta, Ceramics International, Journal of Materials Research, Materials Science & Engineering A, Materials Letters, Journal of Alloys and Compounds, Journal Of Raman Spectroscopy, Materials and Design, Journal of Materials Science & Technology, Journal of Advanced Ceramics, Chemical Engineering Journal, Journal of Physics and Chemistry of Solids, International Journal of Applied Ceramic Technology, Journal of Electronic Materials, Materials Research Express, Solid State Communications, Journal of Micromechanics and Molecular Physics, Physics Scripta.

SKILLS

Theory

Solid Mechanics: Composite Mechanics, Computational Mechanics, Fracture and Damage Mechanics, Experimental Mechanics.

Material Science and Engineering: Computational Material Science (First principle), Ceramic Material Science, Phase stability, Lattice dynamics (phonon).

Experimental techniques

Solid Mechanics: Mechanical tests (Bending, Compression, Fracture toughness, Vickers hardness), thermal shock test.

Material Science and Engineering: Combustion Synthesis (SHS), Thermal and electric property tests, X-ray diffraction (XRD), Scanning electron microscopy (SEM), Transmission electron microscope (TEM).

Numerical modeling

Solid Mechanics: Finite element methods, molecular dynamics.

Material Science and Engineering: Ab initio calculation (CASTEP, VASP)

Computer Language: C, Visual Basic (basic)

Languages: Chinese (native), English (fluent)