

Pengfei Guan

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RESEARCH Computational materials and physics, Glassy materials and physics,
 INTERESTS High-throughput and Machine Learning simulations, and as well as the
 advanced materials design using theory and simulations,

EDUCATION Functional Materials Research Institute, **CISRI**, Beijing, China
 Ph.D. Materials Science, July 2008

Jilin University, Changchun, China
 M.S. Condensed matter physics, July 2003
 B.S. Physics, July 2000

ACADEMIC POSITIONS **2021-present** Full Professor, Beijing CSRC, CHINA
2020-2021 Associate Professor, Beijing CSRC, CHINA
2014-2020 Assistant Professor, Beijing CSRC, CHINA
2011-2014 Postdoctoral Fellow, Johns Hopkins University, USA
2008-2011 Postdoctoral Fellow, Tohoku University, JAPAN
2003-2004 Research Assistant, IOP-CAS, CHINA

AWARDS AND FELLOWSHIPS **2019** Early Career Awards, Computational Material Science
 Branch, CMRS
2018 Outstanding Young Scientist Awards, Amorphous
 Alloy Branch, CMRS
2014 Young “1000-talent”, CHINA

EXTERNAL SUPPORT 2016-2019 ¥0.8M, PI General program, NSFC
 2016-2019 ¥0.5M, co-PI 973 Program, MOST
 2016-2019 ¥0.5M, co-PI General Research Fund, Hong Kong
 2018- ¥20.0M PI “Scientific Challenge Program”, CAEP
 2016- ¥1.5M, PI Joint Programs in CAEP
 2014- ¥3.0M, PI Young “1000-talent” Program

PH.D. Summer 2018 Yuchao Hu IOP-CAS
 SRUDENTS CO- Summer 2018 Bing Wang IOP-CAS
 /SUPERVISED Summer 2018 Qi Liu CSRC (M.S.)
 Summer 2019 Yicheng Wu IOP-CAS

	Summer 2019	Siming An	Tsinghua University
	Summer 2019	Nannan Ren	Shangdong University
	expected 2020	San Zhang	CSRC
	expected 2022	Shengjun Sun	CSRC
	expected 2021	Xurui Wei	CSRC
	expected 2024	Huanrong Liu	CSRC
POSTDOCTORAL ASSOCIATES	2015-2017	Rui Su	Ph.D. Sichuan University
	2015-2019	Lijin Wang	Ph.D. USTC
	2018-2020	Bin Xu	Ph.D. Shanghai Jiaotong University
	2016-	Baoshuang Shang	Ph.D. IOM-CAS
	2019-	Yicheng Wu	Ph.D. IOP-CAS
	2019-	Nannan Ren	Ph.D. Shangdong University
PREPRINTS AND SUBMITTED MANUSCRIPTS	Rui Su, Junping Du, Xuefeng Zhang, Yong Yang, Weihua Wang, <u>Pengfei Guan*</u> , <i>Ultra-slow atomistic simulations revealing the atomic origin of plasticity-brittleness transition in metallic glasses</i> , submitted.		
	Wenxiong Song, Yong Yang, Weihua Wang, <u>Pengfei Guan*</u> , <i>Revealing Rejuvenated Disorder States towards Crystallization in a Supercooled Metallic Glass-Forming Liquid</i> , submitted & under-reviewed by Nature Communications, arXiv:2002.09669		
PEER-REVIEWED PUBLICATIONS	Updated: 2021.05.31 <i>Google scholar:</i> https://scholar.google.com/citations?user=yJi9L7sAAAAJ&hl=zh-CN&oi=ao		

Selected Publications

1. Baoshuang Shang, Weihua Wang, Alan Lindsay Greer, **P. F. Guan***, Atomistic modelling of thermal-cycling rejuvenation in metallic glasses. *Acta Materialis*. 213, 116952(2021)
2. B. Shang, **P. Guan***, J. L. Barrat*, Elastic avalanches reveal marginal behaviour in amorphous solids, *Proc. Natl Acad. Sci.* 117, 86 (2020)
3. B. S. Shang, Jörg Rottler, P. Guan*, J.-L. Barrat*, *Phys. Rev. Lett.* 122,105501 (2019), **Editors' Suggestion**;
4. L. Wang, N. Xu*, W. H. Wang, P. Guan*, *Phys. Rev. Lett.* 120,125502 (2018);
5. Y. C. Hu*, Y. W. Li, Y. Yang, P. Guan*, H. Y. Bai, W. H. Wang, *Proc.*

Natl Acad. Sci. 115, 6375(2018);

6. Y. C. Hu, Y. Z. Wang, R. Su, C. R. Cao, F. Li, C. W. Sun*, Y. Yang, P. Guan*, D. W. Ding, Z. L. Wang, W. H. Wang*, *Adv. Mater.* 28, 10293(2016);
7. P. Guan, S. Lu, M. Spector, P. K. Valavala, M. L. Falk, *Phys. Rev. Lett.* 110, 185502 (2013);
8. P. Guan, T Fujita, A Hirata, Y. H. Liu, M. W. Chen, *Phys. Rev. Lett.* 108, 175501 (2012);
9. A. Hirata, P. Guan, T. Fujita, Y. Hirotsu, A. Inoue, A. R. Yavari, T. Sakurai and M. Chen*, *Nature Materials* 10, 28 (2011);
10. P. Guan, M Chen, T Egami. Stress-temperature scaling for steady-state flow in metallic glasses. *Phys. Rev. Lett.* 104, 205701 (2010).

2021

114. Baoshuang Shang, Weihua Wang, Alan Lindsay Greer, P. F. Guan*, Atomistic modelling of thermal-cycling rejuvenation in metallic glasses. *Acta Materialis*. 213, 116952(2021)
113. Bin Xu, M. L. Falk*, Sylvain Patinet, P. F. Guan*, Atomic nonaffinity as a predictor of plasticity in amorphous solids. *Phys. Rev. Mater.* 5, 025603(2021)
112. P. F. Guan*, S. J. Sun, Atomic-level study in the structure and its instability of metallic glasses. *Acta Metall Sin.* 57, 501-514 (2021). *Invited review*
111. S. J. Sun, P. F. Guan*. The critical model size for simulating the structure-dynamics correlation in bulk metallic glasses. *Sci. China Mater.*, 64, 1545-1555(2021)
110. Nannan Ren, Lina Hu*, Bing Wang, Kaikai Song, Pengfei Guan*. *Scripta Materialia*, 200, 113926 (2021)
109. Z. H. Zhang, W. W. Liu, B. Zhang, B. Sateesh, L. J. Yuan, D. C. Zhu, P. F. Guan, S. J Pennycook, J. J. Guo. Defect-nucleated phase transition in atomically-thin WS₂. *2D Mater.* 8 025017(2021)
108. Y. C. Wu, B. Xu, Y. T. Sun, P. F. Guan*, The quantitative structure-plasticity relationship in metallic glass: a machine learning study, *Chin. Phys.*

B, 30, 057103(2021)

107. J. Guo, S. Q. Zhang, J. Zhang, S. P. Zhou, P. F. Guan. Exploration of electron vortices in the photoionization of diatomic molecules in intense dense fields. *Laser Physics*, 31, 065301 (2021)

106. S. Zhang, W. H. Wang, **P. F. Guan***. Dynamic Crossover in Metallic Glass Nanoparticles. *Chin. Phys. Lett. (Express Letter)* 38, 016802 (2021).

2020

105. D. Richard, M. Ozawa, S. Patinet, E. Stanifer, B. Shang, S. A. Ridout, B. Xu, G. Zhang, P. K. Morse, J.-L. Barrat, L. Berthier, M. L. Falk, **P. Guan**, A. J. Liu, K. Martens, S. Sastry, D. Vandembroucq, E. Lerner, and M. L. Manning. Predicting plasticity in disordered solids from structural indicators. *Phys. Rev. Mater.* 4, 113609 (2020).

104. M. Yu, C. Chen, Q. Liu, C. Mattioli, H. Sang, G. Shi, W. Huang, K. Shen, Z. Li, P. Ding, **P. F. Guan**, S. Wang, Y. Sun, J. Hu, A. Gourdon, L. Kantorovich, F. Besenbacher, M. Chen, F. Song, F. Rosei. Long-range ordered and atomic-scale control of graphene hybridization by photocycloaddition, *Nat. Chem.*, 12, 1035–1041 (2020)

103. W. W. Liu, L. J. Yuan, Z. H. Zhang, X. F. Zhang, **P. F. Guan**, J. T. Sun, S. Bandaru, J. J. Guo. The synergetic effect of straining and N-doping in graphene for enhanced oxygen reduction reaction performance, *Materials Express* 10(10), 1718-1724 (2020).

102. B. Wang, Z. Y. Zhou, **P. F. Guan**, H. B. Yu, W. H. Wang, and K. L. Ngai. Invariance of the relation between α relaxation and β relaxation in metallic glasses to variations of pressure and temperature, *Phys. Rev. B*, 102, 094205 (2020).

101. L. Chen, J. Y. Yu, X. F. Zhang, **P. F. Guan**, R. Su. Theoretical Modeling of Site Selectivity and Chemical Substitution Effect of H₂O₂ Production Efficiency on Modified Graphene, *Catalysis Letters*, 1-8. (2020)

100. Y. X. Li, Y. Zheng, R. Liu, Y. Rao, R. Su, J. Y. Yu, X. G. Liu, **P. F. Guan**, J. J. Guo, X. F. Zhang, G. W. Qin. Enhanced high-frequency microwave absorption in core-shell nanocapsules with atomic-scale oxygen substitutions, *J Appl. Phys.*, 127(19) 195107 (2020)

99. H. Li, P. Liu, Q. Liu, R. Luo, C. G. Guo, Z. Q. Wang, **P. F. Guan**, C. F. Aleman, F. Q. Huang, M. W. Chen. Twisted 1T TaS₂ bilayers by lithiation exfoliation, *Nanoscale*, 12(35) 18031-18038 (2020)

98. Y. H. Gao[#], **P. F. Guan^{#,*}**, R. Su[#], H. W. Chen, C. Yanga, C. He, L. F. Cao, H. Song, J. Y. Zhang, X.F. Zhang, G. Liu*, J. F. Nie, J. Sun*, and E. Ma, *Segregation-sandwiched stable interface suffocates nanoprecipitate coarsening to elevate creep resistance*, [Mater. Res. Lett.](#), 8, 446 (2020)

97. B. Wang, L. J. Wang, B. S. Shang, X. Q. Gao, Y. Yang*, H. Y. Bai, M. X. Pan*, W. H. Wang, P. F. Guan*, *Revealing the low-temperature fast relaxation peak in a model metallic glass*, [Acta Mater.](#) 195, 2611-620(2020)

96. Shan Zhang, Chaoyi Liu, Yong Yang, Yue Fan, **Pengfei Guan***, *Soft Mode Parameter as an Indicator for the Activation Energy Spectra in Metallic Glass*, [J. Phys. Chem. Lett.](#) 11, 2781-2787(2020)

95. N. Ren, L. Hu*, L. Wang*, **P Guan***, *Revealing a hidden dynamic signature of the non-Arrhenius crossover in metallic glass-forming liquid*, [Scripta Materialia](#). 181, 43 (2020);

94. B. Shang, **P Guan***, J. L. Barrat*, *Elastic avalanches reveal marginal behaviour in amorphous solids*, [Proc. Natl Acad. Sci.](#) 117, 86 (2020);

93. H. Chen, S. Zhou*, B. Dong, J. Jin, T. Liu*, **P. Guan***, *A general rule for transition metals doping on magnetic properties of Fe-based metallic glasses*, [Journal of Alloys and Compounds](#), 819, 153062 (2020);

2019

92. Jiang Ma, Can Yang, Xiaodi Liu, Baoshuang Shang, Quanfeng He, Fucheng Li, Tianyu Wang, Dan Wei, Xiong Liang, Xiaoyu Wu, Yunjiang Wang, Feng Gong*, **Pengfei Guan***, Weihua Wang*, Yong Yang*, *Fast surface dynamics enabled cold joining of metallic glasses*, [Science Advances](#) 11, eaax7256 (2019);

91. L Wang, L Berthier, E Flenner*, **P Guan***, G Szamel, *Sound attenuation in stable glasses*, [Soft Matter](#). 15 (35), 7018-7025 (2019);

90. G Chen, J Liu, Q Li, **P Guan**, X Yu, L Xing, J Zhang, R Che, *A direct H₂O₂ production based on hollow porous carbon sphere-sulfur nanocrystal composites by confinement effect as oxygen reduction electrocatalysts*, [Nano Research](#) 12 (10), 2614-2622 (2019);

89. Lihua Wang, Tao Sun, Rujian Wei, **Pengfei Guan**, Pan Liu, Minwei Chen, Ze Zhang, Xiaodong Han, *Bent strain values affect the plastic deformation behaviours of twinned Ni NWs*, [Scripta Materialia](#) 1167, 1 (2019);

88. Longhu Hao, Qi Liu, Yunyi Fang, Ming Huang, Wei Li, Yan Lu, Junfeng Luo, [Pengfei Guan](#), Ze Zhang, Lihua Wang, Xiaodong Han, *Mechanical behavior of metallic nanowires with twin boundaries parallel to loading axis*, [Computational Materials Science](#), 169, 109087 (2019);

87. Qi Liu, Yunhao Zhao, Weiwei Liu, Meiyu Wang, Jingjun Ding, Yuzhang Feng, Wenbin You, Peng Wang, [Pengfei Guan](#), Renchao Che, *Understanding the role of aluminium in determining the surface structure and electrochemical performance of layered cathodes*, [Nanoscale](#) 11, 13007 (2019)

86. B. S. Shang, Jörg Rottler, [P. Guan*](#), J.-L. Barrat*, *Local versus Global Stretched Mechanical Response in a Supercooled Liquid near the Glass Transition*, [Phys. Rev. Lett.](#) 122,105501 (2019), [Editors' Suggestion](#);

85. N. Chen*, D. Wang, [P. Guan](#), H. Y. Bai, W. H. Wang, Z. J. Zhang, H. Hahn, H. Gleiter, *Direct observation of fast surface dynamics in sub-10-nm nanoglass particles*, [Appl. Phys. Lett.](#) 114(4), 043103 (2019)

84. L. Wang, A. Ninarello, [P. Guan*](#), L. Berthier, G. Szamel, E. Flenner*, *Low-frequency vibrational modes of stable glasses*, [Nature Communications](#) 10, 26 (2019)

83. H. L. Liang*, S. J. Cui, R. Su, [P. Guan](#), Y. H. He, L. H. Yang, L. M. Chen, Y. H. Zhang, Z. X. Mei*, X. L. Du, *Flexible X-ray Detectors Based on Amorphous Ga₂O₃ Thin Films*, [ACS Photonics](#) 6,351-359(2019)

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82. Y. C. Hu*, Y. W. Li, Y. Yang, [P. Guan*](#), H. Y. Bai, W. H. Wang, *Configuration correlation governs slow dynamics of supercooled metallic liquids*, [Proc. Natl Acad. Sci.](#) 115, 6375(2018)

81. L. Wang, N. Xu*, W. H. Wang, [P. Guan*](#), *Revealing the Link between Structural Relaxation and Dynamic Heterogeneity in Glass-Forming Liquids*, [Phys. Rev. Lett.](#) 120,125502 (2018)

80. S. M. An, R. Su, S. Zhao, J. Liu*, B. X. Liu, [P. Guan*](#), *Ultrasmall nanoparticles inducing order-to-disorder transition*, [Phys. Rev. B](#) 98(13),134101(2018)

79. A. Hirata, T. Ichitsubo, [P. Guan](#), T. Fujita, M. W. Chen, *Distortion of Local Atomic Structures in Amorphous Ge-Sb-Te Phase Change Materials*, [Phys. Rev. Lett.](#) 120, 205502(2018)

78. C. Y. Liu, P. Guan, Y. Fan, *Correlating defects density in metallic glasses with the distribution of inherent structures in potential energy landscape*, [Acta Mater.](#) 161, 295-301(2018)

77. S. M. An, R. Su, Y. C. Hu, J. B. Liu*, Y. Yang, B. X. Liu, P. Guan*, *Common mechanism for controlling polymorph selection during crystallization in supercooled metallic liquids*, [Acta Mater.](#) 161: 367-373(2018)

76. S. An, Y. Li, J. Li, S. Zhao, B. X. Liu*, P. Guan*, *The linear relationship between diffusivity and crystallization kinetics in a deeply supercooled liquid Ni50Ti50 alloy*, [Acta Mater.](#) 152, 1-6(2018)

75. N. Ren, B. S. Shang, P. Guan*, L. Hu*, *General structural and dynamic characteristics beneficial to glass-forming ability of Fe-based glass-forming liquids*, [J. Non-Cryst. Solids](#) 481,116-122(2018)

74. B. Jia, Z. Guan, Z. Peng, J. Zhang, X. Guan, P. Guan, B. Yang*, Y. Wang, P. Lu*, *Structural disorder in fused silica with ODC (I) defect*, [Appl. Phys. A](#) 124(10): 696(2018)

73. L. Sun, Z. Li, R. Su, Y. Wang, Z. Li, B. Du, Y. Sun*, P. Guan*, F. Besenbacher*, M. Yu*, *Phase-transition induced conversion to photothermal material: Quasi-metallic WO₂. 9 nanorods for solar water evaporation and anticancer photothermal therapy*, [Angew. Chem. Int. Edit.](#) 57(33):10666-10671(2018)

72. Z. Mao, H. Hu, R. Su, P. Liu, Y. Li, W. Zhang, X. Zhao, J. Guo, P. Guan, G. Qin, X. F. Zhang*, *Cover Feature: Confining Gold Nanoclusters in Highly Defective Graphitic Layers To Enhance the Methanol Electrooxidation Reaction*, [ChemCatChem](#) 10(1), 141-147(2018)

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70. B. S. Shang, P. Guan*, J.-L. Barrat*, *Role of thermal expansion heterogeneity in the cryogenic rejuvenation of metallic glasses*, [J. Phys. Mater.](#) 1(1), 15001(2018)

69. L. Wu, Q. Wang, C. Yang, R. Quhe, P. Guan, P. Lu*, *Crown oxygen-doping graphene with embedded main-group metal atoms*, [Eur Phys J B](#) 91(2), 46(2018)

68. Q. Liu, P. Guan*, *First principle study on atomic structure of La₆₅X₃₅ (X = Ni, Al) metallic glasses*, *Acta Physica Sinica* 67(17), 178101(2018)

67. Q. Wang, R. Quhe, Z. Guan, L. Wu, J. Bi, P. Guan, M. Lei, P. Lu, *High n-type and p-type thermoelectric performance of two-dimensional SiTe at high temperature*, *RSC Adv.* 8(38), 21280-21287(2018)

66. M. Li, W. Liu, H. Zhang, Z. Liang, P. Duan, X. Yan, P. Guan, B. S. Xu, J. Guo*, *Direct imaging of construction of carbon onions by curling few-layer graphene flakes*, *Phys. Chem. Chem. Phys.* 20(3), 2022-2027(2018)

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64. L. Wu, P. Lu, R. Quhe, Q. Wang, C. Yang, P. Guan, K. Yang, *Stanene nanomeshes as anode materials for Na-ion batteries*, *J. Mater. Chem. A* 6(17): 7933-7941(2018)

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61. S. Ma, B. Wurentuya, X. X. Wu, Y. J. Jiang, O. Tegus, P. Guan, B. Narsu*, *Ab initio mechanical and thermal properties of FeMnP_{1-x}Gax compounds as refrigerant for room-temperature magnetic refrigeration*, *RSC Adv.* 7(44),27454-27463(2017)

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H. L. Xu*, R. C. Che*, *Simultaneous Ni doping at atom scale in ceria and assembling into well-defined lotuslike structure for enhanced catalytic performance*, [ACS appl. Mater. Inter.](#) 9(19): 16243-16251(2017)

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56. C. J. Ruan, L. H. Han, X. Chen, X. C. Li, C. F. Zhang, P. F. Lu*, [P. Guan*](#), *First Principles Calculations of Electronic Properties on M₁₃Pt₄₂ (M= Al, Ga, In, Mg, Ca, Sr)*, [J. Clust. Sci.](#) 28(3), 1749-1759(2017)

55. Y. C. Hu, [P. Guan*](#), Q. Wang, Y. Yang*, H. Y. Bai, W. H. Wang*, *Pressure effects on structure and dynamics of metallic glass-forming liquid*, [J. Chem. Phys.](#) 146(2): 24507(2017)

54. B. Wang, L. J. Wang, W. H. Wang, H. Y. Bai, X. Q. Gao, M. X. Pan*, [P. Guan*](#), *Understanding the maximum dynamical heterogeneity during the unfreezing process in metallic glasses*, [J Appl. Phys.](#) 121, 175106(2017)

53. P. Lu, L. Y. Wu, C. H. Yang, D. Liang, R. Quhe*, [P. Guan*](#), S. Wang, *Quasiparticle and optical properties of strained stanene and stanane*, [Sci. Rep.](#) 7, 3912(2017)

52. D. Liang, R. Quhe*, Y. J. Chen, L. Wu, Q. Wang, [P. Guan*](#), S. M. Wang, P. F. Lu*, *Electronic and excitonic properties of two-dimensional and bulk InN crystals*, [RSC Adv.](#) 7, 42455-42461(2017)

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50. Y. C. Wu, B. Wang, Y. C. Hu, Z. Lu, Y. Z. Li, B. S. Shang, W. H. Wang, H. Y. Bai*, [P. Guan*](#), *The critical strain-A crossover from stochastic activation to percolation of flow units during stress relaxation in metallic glass*, [Scripta Mater.](#) 134, 75-79(2017)

49. L. H. Wang#, [P. Guan#](#), J. Teng, P. Liu, D. K. Chen, W. Xie, D. Kong, S. B. Zhang, T. Zhu, Z. Zhang, *New twinning route in face-centered cubic nanocrystalline metals*, [Nat. Commun.](#) 8(1): 2142(2017)

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oxidation of carbon nanotubes, [Nature Communications](#) 7,12251(2016)

47. L. Zhang, H. W. Liu, L. Y. Chen, **P. Guan**, B. Chen, T. Fujita, Y. Yamaguchi, H. Iwasaki, Q. K. Xue, M. W. Chen*, *Large-scale growth of sharp gold nano-cones for single-molecule SERS detection*, [RSC Adv.](#) 6(4), 2882-2887(2016)

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40. X. C. Li, X. Chen, L. H. Han, C. J. Ruan, P. F. Lu*, **P. Guan***, *First-principles study of the structural, elastic and electronic properties of Pt3M alloys*, [J. Mater. Res.](#) 31(19), 2956--2963(2016)

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35. B. Wang, B. S. Shang, X. Q. Gao, W. H. Wang, H. Y. Bai, M. X. Pan*, P. Guan*, *Understanding Atomic-Scale Features of Low Temperature-Relaxation Dynamics in Metallic Glasses*, [J. Phys. Chem. Lett.](#) 7(23), 4945-4950(2016)

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33. X. F. Zhang*, J. J. Guo, P. Guan*, G. W. Qin*, S. J Pennycook, *Gigahertz dielectric polarization of substitutional single niobium atoms in defective graphitic layers*, [Phys. Rev. Lett.](#) 115, 147601(2015)

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2. L. G. Cong, T. M. He*, Y. Ji, [P. Guan](#), Y. L. Huang, W. H. Su, *Synthesis and characterization of IT-electrolyte with perovskite structure La_{0.8}Sr_{0.2}Ga_{0.85}Mg_{0.15}O_{3-delta} by glycine-nitrate combustion method*, [Journal of Alloys and Compounds](#) 348,325-331(2003)

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1. T. M. He*, Z. Lu, Y. L. Huang, [P. Guan](#), J. Liu, W. H. Su, *Characterization of YSZ electrolyte membrane tubes prepared by a vacuum casting method*, [Journal of Alloys and Compounds](#) 337,231-236(2002)

SELECTED
INVITED TALKS

2019 Plenary lecture, The 2019 International Conference on Multi-scale Modeling & Simulation of Materials (ICM3-2019)

- 2019 Invited Talk, C-MRS Meeting, @Chengdu
 - 2019 Invited Talk, The 4th Sino-German workshop on “Universal Aspects of Disordered Systems – the Generic Cases of Metallic Glasses and Colloids”, @German
 - 2018 Invited Talk, The 2018 International Conference on Multi-scale Modeling & Simulation of Materials (ICM3-2018), 2018@Xi’an
 - 2017 Invited Talk, the 8th International Discussion Meeting on Relaxations in Complex Systems (8IDMRCS), 2017@Poland
 - 2017 Invited Talk, C-MRS Meeting, @Dalian
 - 2016 Invited Talk, THERMEC’2016, 2016@Austria
 - 2016 Invited Talk, C-MRS Meeting, @Dalian
 - 2016 Invited Talk, The 11th International Conference of Bulk Metallic Glasses (BMG XI), @St. Louis
 - 2015 Invited Talk, C-MRS Meeting, @Guiyang
 - 2014 Invited Talk, The 2nd International Conference of Young Researchers on Advanced Materials, C-MRS, October 2014@Haikou
- + **20+ talks prior**

TEACHING

Graduate School of CAEP

Spring 2020, Spring 2019,

Spring 2018, Spring 2017

Foundation of Materials Science

PROFESIONAL

- NSFC Reviewer

ACTIVITIRS AND
OUTREACH

- 2016 Amorphous Materials and Application Branch of Chinese Society for Metals, Committee *member*
- 2016 Computational Materials Science Branch of CMRS, Committee *member*
- 2020 Co-organizer and co-chair, APS March Meeting Focus Topic on “Understanding Glasses and Disordered Matter Through Computational Models”
- 2018 Organizer and Chair, *International mini-Workshop / Summer School on Structure and Instability of Amorphous Materials*
- 2017 Co-organizer and co-chair, *International Conference on Algorithms and Applications for Excited State Electronic Structure Theories*
- 2017 Organizer and co-Chair, *Advanced Training Class/Workshop--New materials exploration and design based on multi-scale high throughput simulations*
- 2016 Chair, Symposiums on Amorphous materials related to the *CAEP Strategic Development Plan of Materials Science*