

# *CURRICULUM VITAE*

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## PROFESSIONAL POSITIONS

2012/07-present Associate researcher, Institute of High Energy Physics, Chinese Academy of Sciences  
2010/07- 2012/07 Assistant researcher, Institute of High Energy Physics, Chinese Academy of Sciences  
2012/06-2012/08 Visiting Scientist, Brookhaven National Laboratory, US.  
2012/08-2012/12 Visiting Scientist, Argonne National Laboratory, US.

## EDUCATION

2005-2010 Ph.D. Condensed Matter Physics, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing  
Advisor: Prof. Ziyu Wu  
Thesis Title: "Application of X-ray Absorption Spectroscopy and First Principles on Functional materials"  
  
2008.2-2008.12 Fellowship scholar, Laboratori Nazionali di Frascati, Istituto Nazionale di Fisica Nucleare, Rome  
Advisor: Prof. Augusto Marcelli  
Project Title: "Conceptual design of an Infrared and X-ray Simultaneous Spectroscopy beamline"  
  
2001-2005 B.S. Materials Physics, Harbin University of Science and Technology, Harbin

## RESEARCH INTERESTS

- ✧ Materials sciences, in particular on those with complex atomic, electronic structures
- ✧ X-ray absorption fine-structure spectroscopy, both in experiments and theoretical simulations.
- ✧ X-ray Fluorescence spectroscopy and microscopic mapping
- ✧ Synchrotron optics including crystals and novel mirrors
- ✧ Infrared spectroscopy/microscopy, complex 2d correlation analysis
- ✧ First principles calculations based on density functional theory

## MILESTONE PROJECTS

**Team leader** of the R&D of high energy resolution monochromator at 14 keV, subprojects of the National R&D Projects for High Energy Photon Source in China, **2013-2016**  
**Principle investigation** of "Local structure and transport property relationship of misfit layered  $\text{Ca}_3\text{Co}_4\text{O}_9$  based thermoelectric materials", *National Science Foundation of China*, Grant No.11105172, **2012-2014**  
**Principal participants** in the conceptual beamline design of the combinatorial simultaneous X-ray and infrared spectroscopy, with a close collaboration with Dr. Augusto Marcelli **2008-2010**

## PUBLICATIONS

- [1] **W. Xu**, K. Dziejcz-Kocurek, M. Yu, Z. Wu and A. Marcelli, Spectroscopic study and electronic structure of prototypical iron porphyrins and their [small mu ]-oxo-dimer derivatives with different functional configurations, *RSC Advances*, 4, 46399-46406. (2014)
- [2] **W. Xu**,\* Y. Liu, B.Chen, D. Liu, Y. Lin and A. Marcelli, Nano-inclusions: a novel approach to tune the thermal conductivity of the  $\text{In}_2\text{O}_3$ , *Phys. Chem. Chem. Phys.*, **15**, 17595-17600 (2013)
- [3] **W. Xu**,\* Y. Liu, L. Zhao, P. An, Y. Lin, M. Augusto and Z. Wu, Evidence of an interlayer charge transfer route in  $\text{BiCu}_{1-x}\text{SeO}$ , *Journal of Materials Chemistry A*, **1**, 12154-12158 (2013)
- [4] **W. Xu**,\* L.J. Liu, M.Q. Cui, L. Zheng, Y. F. Hu, A. Marcelli and Z. Y. Wu, Electronic structure and hybridization of CaS by means of X-ray absorption spectroscopy at Ca and S K-edges, *Journal of Synchrotron Radiation*, 20, 110-115 (2013)
- [5] **W. Xu**,\* X.L. Zhang, Z.Y. Guo, C. Si, Y.D. Zhao, A. Marcelli, D.L. Chen, and Z.Y. Wu, Copper L-edge spectra: multiplet vs. multiple scattering theory, *Journal of Physics: Conference Series*, 430, 012010 (2013)
- [6] **W. Xu**,\* A. Marcelli, L. Liu, C.R. Wang, Z. Y. Wu, Endohedral fullerenes: a concurrent characterization by means of synchrotron radiation X-ray and IR spectroscopy, *Journal of Physics: Conference Series*, 430, 012069 (2013)
- [7] **W. Xu**, A. Marcelli, D. Hampai, L. Malfatti, P. Innocenzi, U. Schade and Z. Wu, New opportunity to investigate physico-chemical phenomena: time-resolved X-ray and IR concurrent analysis, *Rendiconti Lincei*, 22, S59-S79. (2011)
- [8] **W. Xu**, Y. Liu, D. Chen, Y.-H. Lin, Z. Wu, Y. Xie, B.-P. Zhang, B. Cheng, C.-W. Nan and Z. Wu, High Temperature Transport Property of Copper site Doped  $\text{La}_2\text{CuO}_4$ , *Journal of the American Ceramic Society*, 94, 1471-1476. (2011)
- [9] **W. Xu**, D. Chen, W. Chu, Z. Wu, A. Marcelli, A. Mottana, A. Soldatov and M. F. Brigatti, Quantitative local structure determination in mica crystals: ab initio simulations of polarization XANES at the potassium K-edge, *Journal of Synchrotron Radiation*, 18, 418-426. (2011)
- [10] **W. Xu**, A Marcelli, B Joseph, A Iadecola, W S Chu, D Di Gioacchino, A Bianconi, Z. Y. Wu and N. L. Saini, Arsenic K-edge XANES study of  $\text{REFeAsO}$  oxypnictides, *EPL (Europhysics Letters)*, 90, 57001. (2010)
- [11] **W. Xu**, A Marcelli, B Joseph, A Iadecola, W S Chu, D Di Gioacchino, A Bianconi, Z. Y. Wu and N. L. Saini, Local structural disorder in  $\text{REFeAsO}$  oxypnictides by RE L3 edge XANES, *Journal of Physics: Condensed Matter*, 22, 125701. (2010) (IOP select)
- [12] Y. Liu, **W. Xu**, D.B. Liu, M. J. Yu, Y. H. Lin and C. W. Nan, Enhanced thermoelectric properties of Ga-doped  $\text{In}_2\text{O}_3$  ceramics via synergetic band gap engineering and phonon suppression, *Phys. Chem. Chem. Phys.*, 2015, DOI: 10.1039/C5CP00739A
- [13] S. Butt, **W. Xu**, M. U. Farooq, G. K. Ren, F. Mohamed, Y. Lin and C.-W. Nan, Enhancement of Thermoelectric Performance in Hierarchical Mesoscopic Oxide Composites of  $\text{Ca}_3\text{Co}_4\text{O}_9$  and  $\text{La}_{0.8}\text{Sr}_{0.2}\text{CoO}_3$ , *J. Am. Ceram. Soc.*, (2015) DOI: 10.1111/jace.13459
- [14] S. Butt, **W. Xu**\*, W. Q. He, Q. Tan, G. K. Ren, Y. Lin and C. Nan, Enhancement of thermoelectric performance in Cd-doped  $\text{Ca}_3\text{Co}_4\text{O}_9$  via spin entropy, defect chemistry and phonon scattering, *Journal of Materials Chemistry A*, 2, 19479-19487, (2014)
- [15] J. Cheng, **W. Xu**, L. Liu, P. Dong and S. Liu, Heterogeneous Structural Distortions Induced by In-Plane and Out-of-Plane Doping in Iron-Based Superconductors, *J Supercond Nov Magn*, 1-5. (2014)
- [16] M. Huang, **W. Xu**, Y. Shen, Y.-H. Lin, C-W. Nan, X-ray absorption near-edge spectroscopy study on Ge-doped  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ : enhanced ionic conductivity and defect chemistry, *Electrochim. Acta*, 115, 581-586. (2014)
- [17] C. Si, **W. Xu**, H. Wang, J. Zhou, A. Ablat, L. Zhang, J. Cheng, Z. Pan, L. Fan, C. Zou and Z. Wu, Metal-insulator transition in  $\text{V}_{1-x}\text{W}_x\text{O}_2$ : structural and electronic origin, *Physical Chemistry Chemical Physics*, 14, 15021-15028. (2012)
- [18] T. Zhao, **W. Xu**, Q. Ye, J. Cheng, H. Zhao, Z. Wu, D. Xia and W. Chu, Local structure of vanadium in doped  $\text{LiFePO}_4$ , *Journal of Synchrotron Radiation*, 17, 584-589. (2010)
- [19] Marcelli, **W. Xu**, D. Hampai, L. Malfatti, P. Innocenzi, U. Schade and Z. Wu, Infrared and X-ray simultaneous spectroscopy: a novel conceptual beamline design for time resolved experiments, *Analytical and Bioanalytical Chemistry*, 397, 2095-2108-2108. (2010)
- [20] Marcelli, **W. Xu**, L. Liu, C. Wang, W. Chu and Z. Wu, Dynamical behavior in  $\text{C}_{82}$  metal endohedral fullerenes: 2D correlation analysis of x-ray and infrared data, *Journal of Nanophotonics*, 3, 031975-031979. (2009)

- [21] H. X. Wang, C. H. Zhou, **W. Xu**, Synchrotron radiation based nuclear resonant vibrational spectroscopy: Introduction, *WuLi*, 43, 579-588. (2014) (In chinese)
- [22] H. X. Wang, C. H. Zhou, **W. Xu**, Synchrotron radiation based nuclear resonant vibrational spectroscopy: Applications, *WuLi*, 43, 640-649. (2014) (In chinese)
- [23] W. Jiang, Q. Cai, **W. Xu**, M. Yang, Y. Cai, D. D. Dionysiou and K. E. O'Shea, Cr(VI) Adsorption and Reduction by Humic Acid Coated on Magnetite, *Environmental Science & Technology*, 48, 8078-8085. (2014)
- [24] Y. Liu, J. Lan, **W. Xu**, \* Y. Liu, Y. L. Pei, B. Cheng, D. B. Liu, Y. H. Lin and L. D. Zhao, Enhanced thermoelectric performance of a BiCuSeO system via band gap tuning, *Chem. Commun.*, 49, 8075-8077. (2013)
- [25] Y-H. Lin, W. Deng, **W. Xu**, Y. Liu, D.L. Chen, X.L. Zhang, and C.W. Nan, Abnormal dielectric behaviors in Mn-doped  $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$  ceramics and their response mechanism, *Materials Science and Engineering: B* 177 (20), 1773 (2012).
- [26] Y. Liu, Y.-H. Lin, **W. Xu**, B. Cheng, J. Lan, D. Chen, H. Zhu and C.-W. Nan, High-Temperature Transport Property of  $\text{In}_{2-x}\text{Ce}_x\text{O}_3$  ( $0 \leq x \leq 0.10$ ) Fine Grained Ceramics, *Journal of the American Ceramic Society*, 95, 2568-2572. (2012)
- [27] Marcelli, D. Hampai, **W. Xu**, L. Malfatti and P. Innocenzi, Time Resolved IR and X-Ray Simultaneous Spectroscopy: New Opportunities for the Analysis of Fast Chemical-Physical Phenomena in Materials Science, *Acta Physica. Polonica. A*, 115, 489-500. (2009)
- [28] N.Poccia, M. Chorro, A. Ricci, **W. Xu**, A. Marcelli, G. Campi and A. Bianconi, Percolative superconductivity in  $\text{La}_2\text{CuO}_{4.06}$  by lattice granularity patterns with  $\mu\text{XANES}$  scanning, *Appl. Phys. Lett.* 104, 221903 (2014)
- [29] P. An, C. Hong, J. Zhang, **W. Xu**, and T. Hu, (2014). A facile heating cell for in situ transmittance and fluorescence X-ray absorption spectroscopy investigations. *Journal of Synchrotron Radiation*, 21, 165-169. (2014)
- [30] J. Cheng, P. Dong, W. Chu, **W. Xu**, H. Wen, A. Marcelli and Z. Wu, Strikingly dissimilar effect of Mn and Zn dopants imposed on local structural distortion of  $\text{Ba}_{0.5}\text{K}_{0.5}\text{Fe}_2\text{As}_2$  superconductor, *Journal of Synchrotron Radiation*, 20, 455-459. (2013)
- [31] J. Cheng, J. Zhou, R. Hu, **W. Xu**, Y. Li, L. Zhang, A. Marcelli, W. Chu, Z.-A. Xu and Z.Y. Wu, Charge redistribution and local lattice structure of (F, Zn)-codoped  $\text{LaFeAsO}$  superconductor, *New Journal of Physics*, 14, 033005. (2012)
- [32] J. Cheng, S. Chu, W. Chu, **W. Xu**, J. Zhou, L. Zhang, H. Zhao, R. Liu, X. Chen, A. Marcelli and Z. Wu, Quantum critical point in  $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$  and oxygen vacancy induced by high fluorine dopant, *Journal of Synchrotron Radiation*, 18, 723-727. (2011)
- [33] A. Ricci, B. Joseph, N. Poccia, **W. Xu**, D. Chen, W. S. Chu, Z. Y. Wu, A. Marcelli, N. L. Saini and A. Bianconi, On the possibility of a new multiband heterostructure at the atomic limit made of alternate  $\text{CuO}_2$  and  $\text{FeAs}$  superconducting layers, *Superconductor Science and Technology*, 23, 052003. (2010)
- [34] Y. Liu, Y.-H. Lin, J. Lan, **W. Xu**, B.-P. Zhang, C.-W. Nan and H. Zhu, Effect of Transition-Metal Cobalt Doping on the Thermoelectric Performance of  $\text{In}_2\text{O}_3$  Ceramics, *Journal of the American Ceramic Society*, 93, 2938-2941. (2010)
- [35] N.Poccia, M. Chorro, A. Ricci, **W. Xu**, A. Marcelli, G. Campi and A. Bianconi, Percolative superconductivity in  $\text{La}_2\text{CuO}_{4.06}$  by lattice granularity patterns with  $\mu\text{-XANES}$  scanning, *Appl. Phys. Lett.* 104, 221903 (2014)
- [36] S.-B. Xi, M.-Q. Cui, J.-T. Zhu, D.-L. Yang, **W. Xu**, L.-J. Liu, Z.-Y. Guo, and J. Zhao, An analytical model for the polarization of synchrotron radiation in a soft X-ray region, *Chinese Physics C* 37 (3), 038002 (2013).
- [37] S.-B. Xi, M.-Q. Cui, X.-F. Qin, X.-H. Xu, **W. Xu**, L. Zheng, J. Zhou, L.-J. Liu, D.-L. Yang and Z.-Y. Guo, Origin of Ferromagnetism in  $\text{Zn}_{1-x}\text{Co}_x\text{O}$  Thin Films: Evidences Provided by Hard and Soft X-Ray Absorption Spectroscopy, *Chinese Physics Letters*, 29, 127804 (2012).
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- [42] T. Zhao, W. S. Chu, H. Zhao, X. Liang, **W. Xu**, M. Yu, D. Xia and Z. Wu, XAS study of  $\text{LiFePO}_4$  synthesized by solid

- state reactions and hydrothermal method, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 619,122-127 (2010).
- [43] Marcelli, M. C. Guidi, M. Piccinini, P. Innocenzi, L. Malfatti and **W. Xu**, Synchrotron radiation – a brilliant source for solid-state research in the infrared energy domain, *physica status solidi (c)*, 6, 1999-2007. (2009)
- [44] L.-J. Zhang, J.-Q. Wang, J. Li, J. Zhou, W.-P. Cai, J. Cheng, **W. Xu**, G. Yin, X. Wu, Z. Jiang, S. Zhang and Z.-Y. Wu, High-Tc ferromagnetism in a Co-doped ZnO system dominated by the formation of a zinc-blende type Co-rich ZnCoO phase, *Chemical Communications*, 48, 91-93.(2012).
- [45] J. L. Lan, Y. C. Liu, B. Zhan, Y. H. Lin, B. Zhang, X. Yuan, W. Zhang, **W. Xu** and C. W. Nan, Enhanced Thermoelectric Properties of Pb-doped BiCuSeO Ceramics, *Advanced materials*, 25, 5086-5090 (2013)
- [46] Marcelli, P. Innocenzi, L. Malfatti, M.A. Newton, J. V. Rau, E. Ritter, U. Schade and **W. Xu**, IR and X-ray time resolved simultaneous experiments: an opportunity to investigate the dynamics of complex systems and non-equilibrium phenomena using 3rd generation synchrotron radiation sources, *Journal of Synchrotron Radiation*, 19, 892-904. (2012)
- [47] X. Jiang, J. Wang, Q. Qin, Y. Dong, W. Sheng, J. Cheng, G. Xu, T. Hu, H. Deng, F. Chen, F. Long, H. Lu, J. Yue, C. Li, Y. Sun, J. Chen, H. Dong, Q. Cai, **W. Xu**, M. Li, G. Chang, H. Zheng, Y. Tao, P. Liu, J. Liu, D. Sun, G. Li, H. Shi and J. Cao, The Chinese High-Energy Photon Source and its R&D Project, *Synchrotron Radiation News*, 27, 27-31. (2014)

## **POSTERS**

- [1] Infrared and X-ray simultaneous spectroscopy: a beamline for time resolved simultaneous analysis of physical-chemical processes  
**W. Xu**, A. Marcelli , D. Hampai , L. Malfatti , P. Innocenzi and Z.Y. Wu  
10<sup>th</sup> International Conference on Synchrotron Radiation Instrumentation, Melbourne, Australia, September 27 – October 2, 2009
- [2] A novel beamline of infrared and X-ray simultaneous spectroscopy: opportunities unraveling new sciences  
**W. Xu** , A. Marcelli , D. Hampai , L. Malfatti , P. Innocenzi and Z.Y. Wu  
Local distortions and Physics of Functional materials (LPF09), Rome, Italy, July 22-24, 2009
- [3] Quantitative local structure determination of mica crystals: ab initio simulations of polarized XANES at the potassium K-edge  
**W. Xu**, D. L. Chen, A. Marcelli, A. Mottana, M.F. Brigatti, W. S. Chu, Z.Y. Wu  
21<sup>st</sup> International conference on x-ray and inner-shell processes, Paris, France, June 22 - 27, 2008
- [4] The limits of the muffin-tin approximation for XANES simulations of highly anisotropic systems  
**W. Xu**, D Chen, W Chu, Z Wu, A Soldatov, A Mottana, MF Brigatti, A Marcelli  
37<sup>th</sup> International conference on vacuum ultraviolet and x-ray physics, UBC, Vancouver, Canada July 11-16, 2010
- [5] IR and X-ray simultaneous spectroscopy: a novel framework for time resolved simultaneous analysis of physical-chemical processes  
A Marcelli, **W. Xu**, P Innocenzi, L Malfatti, D Hampai, U Schade, Z Wu  
37<sup>th</sup> International conference on vacuum ultraviolet and x-ray physics, UBC, Vancouver, Canada July 11-16, 2010
- [6] Cr (VI) adsorption and reduction by humic acid coated magnetite: Surface structure.  
W.J. Jiang, Q. Cai, **W. Xu**, D. Dionysiou, K.E. O’Shea.  
The 245<sup>th</sup> ACS National Meeting. New Orleans, LA, USA, April 19-23, 2013.
- [7] Copper L-edge spectra: multiplet vs. multiple scattering theory  
**W. Xu**, X.L. Zhang, Z.Y. Guo, C. Si, Y.D. Zhao, A. Marcelli, D.L. Chen, and Z.Y. Wu  
The 15<sup>th</sup> International Conference on X-ray Absorption Fine Structure, Beijing, China, July 22-28, 2012
- [8] Endohedral fullerenes: a concurrent characterization by means of synchrotron radiation X-ray and IR spectroscopy  
**W. Xu**, A. Marcelli, L. Liu, C.R. Wang, Z. Y. Wu,  
The 15<sup>th</sup> International Conference on X-ray Absorption Fine Structure, Beijing, China, July 22-28, 2012
- [9] Local configurations and charge transfer mechanisms in heme structures of iron porphyrins  
**W. Xu**, K. Dziejcz-Kocurek, A. Marcelli  
38<sup>th</sup> International conference on Vacuum Ultraviolet and X-ray Physics, Hefei, Anhui Province, China, 12-19 July, 2013
- [10] Ray-tracing of nested meV-resolved monochromator: pitfalls and solutions

**W. Xu**, Y. Cai, A. Marcelli, T.D. Hu and Z.Y Wu

38<sup>th</sup> International conference on Vacuum Ultraviolet and X-ray Physics, Hefei, Anhui Province, China, 12-19 July, 2013

[11] Can XANES identify silica oligomers structures?

**W. Xu**, A. Marcelli, G. Cinque, L. Malfatti and P. Innocenzi

38<sup>th</sup> International conference on Vacuum Ultraviolet and X-ray Physics, Hefei, Anhui Province, China, 12-19 July, 2013

[12] Cr(VI) adsorption and reduction by humic acid coated magnetite

Wenjun Jiang, Quan Cai, **Wei Xu**, Yong Cai, Dionysios D. Dionysiou, Kevin E. O'Shea. San Diego.

The 19th International Conference on Advanced Oxidation Technologies for Treatment of Water, Air and Soil., CA, November 17-21, 2013.

[13] Local structure and dynamics of iron-porphyrin complexes: a theoretical and experimental XAS investigation

K. Dziejczak-Kocurek, **Wei Xu** and A. Marcelli

International Congress on X-Ray Optics and Microanalysis, Hamburg, Germany, September 2-6, 2013

## **ORAL PRESENTATIONS**

*High temperature transporting behavior of copper site doped La<sub>2</sub>CuO<sub>4</sub>*

**Local distortions and Physics of Functional materials (LPF09)** Rome Italy, July 22<sup>nd</sup>-24<sup>th</sup>, 2009

*New opportunity to investigate physico/chemical phenomena: time resolved X-ray and IR concurrent analysis*

**1<sup>st</sup> Bilateral Italian/Chinese Workshop on Synchrotron Radiation Time Resolved Concurrent Experiments: Advantages and Future Applications** Shanghai China, November 11<sup>th</sup>, 2010

*Infrared and X-ray Simultaneous Spectroscopy: beamline design and applications*

**1<sup>st</sup> National Annual User Meeting of Chinese large scientific infrastructures**, Beijing, Aug.25<sup>th</sup>- 26<sup>th</sup>, 2011

*Summary on Nuclear Resonant Scattering techniques and design of High Energy Resolution Monochromator*

**Sector 3, Advanced Photon Source, Argonne National Laboratory**, Chicago, Dec.7<sup>th</sup>, 2012

*Enhancement of thermoelectric performance of calcium cobaltite by local misfit structures*

**2<sup>nd</sup> National Annual User Meeting of Chinese large scientific infrastructures**, Shanghai, Aug. 21<sup>st</sup>- 22<sup>nd</sup>, 2013

*Introduction to the High Energy Photon Source of China*

Seminar talk at Dalian Institute of Chemical Physics, Aug.13-Aug.16, 2014

*The era of light: shining the structural and dynamic aspects of energy-related materials*

Seminar talk at Guangxi University, Nov.11-Nov.12, 2014

## **ACADEMIC MEMBERSHIP**

International X-ray Absorption Society

## **SCIENTIFIC ACTIVITIES**

Referees for *Surface Review and Letters*; *International Journal of Modern Physics B*; *X-ray spectrometry*; *Journal of Physics and Chemistry of Solids*, etc.