Yuanpeng Zhang, PhD

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SUMMARY

I love physics, for its beauty of explaining not only the world, but also our life. I love programming, not only for the convenience coming with it, but also for exploring the otherwise untouchable world without it.

I have been using X-ray absorption spectrscopy to characterizate both amorphous and nano-structured systems during my PhD. The early work involves the combined X-ray absorption and scattering analysis for local structure of Ge quantum dots at ambient condition and under hydrostatic pressure.

After I moved to ORNL starting my postdoc, I have been working on using and developing RMCProfile for modeling total scattering data with the 'big-box' approach. Meanwhile, I have been working on several research projects, including the negative thermal expansion coupled with magnetic ordering, the clustering behavior of spin glass system, structure-property relationship in battery materials, etc.

EDUCATION

- **Beihang University**   BEIJING, P. R. CHINA
  Bachelor degree in Physics and Nuclear Energy Engineering   *2008 – 2012*

- **Queen Mary, University of London**   LONDON, UNITED KINGDOM
  PhD degree in Condensed Matter and Materials Physics   *2012 – 2016*
  > ***PhD Thesis:*** Local structure characterization of amorphous and nanoscale systems using X-ray Absorption Spectroscopy (XAS)

EMPLOYMENT

- **Oak Ridge National Laboratory**   OAK RIDGE, UNITED STATES
  Postdoc Research Assistant   *2017 – 2019*

- **National Institute of Standards and Technology**   Maryland, United States
  &
  Oak Ridge National Laboratory   OAK RIDGE, UNITED STATES
  Visiting Scientist   *2019 – Now*

SELECTED PUBLICATIONS

- **Y. P. Zhang***, M. McDonnell, W. Liu and M. G. Tucker*. Reverse Monte Carlo modeling for low-dimensional systems, *J. Appl. Cryst.*, 2019, **52**, 1035-1042.

- **Y. P. Zhang***, M. McDonnell, S. A. Calder and M. G. Tucker*. Mechanistic Insights into the Superexchange-Interaction-Driven Negative Thermal Expansion in CuO, *J. Am. Chem. Soc.*, 2019, **141**, 6310-6317.

- **Y. P. Zhang**, T. Scholz, R. Dronskowski*, M. McDonnell and M. G. Tucker*. Local magnetic cluster size identified by neutron total scattering in the site-diluted spin glass SnxFe4-xN (x=0.88). *Phys. Rev. B*, 2019, **100**, 014419.

- J. X. Hu*, T. H. Huang*, **Y. P. Zhang**, B. Hu, H. Q. Ye, B. J. Chen, H. P. Xia and C. Y. Ji. Enhanced deep-red emission from Mn4+/Mg2+ co-doped CaGdAlO4 phosphors for plant cultivation. *Dalton Trans.*, 2019, **48**, 2455-2466.

- J. X. Hu, **Y. P. Zhang**, H. P. Xia*, H. Q. Ye, B. J. Cheng and Y. S. Zhu. NIR Downconversion and Energy Transfer Mechanisms in Tb3+/Yb3+ Codoped Na5Lu9F32 Single Crystals. *Inorg. Chem.*, 2018, **57**, 7792-7796.

- M. Y. Song*, A. Karatutlu, I. Ali, O. Ersoy, Y. Zhou, Y. X. Yang, **Y. P. Zhang**, W. R. Little, A. P. Wheeler and A. V. Sapelkin. Spectroscopic super-resolution fluorescence cell imaging using ultra-small Ge quantum dots, *Opt. Express*, 2017, **25**, 4240-4253.

- **Y. P. Zhang**, O. Ersoy, A. Karatutlu and A. Sapelkin*.Local structure of amorphous and nanoscale systems by numerical XANES analysis, *J. Non-Cryst. Solids*, 2016, **451**, 10-15.

- A. Karatutlu*, W. Little, O. Ersoy, **Y. P. Zhang**, I. Seker and A. Sapelkin. Laser-induced particle size tuning and structural transformations in germanium nanoparticles prepared by stain etching and colloidal synthesis route, *J. Appl. Phys.*, 2015, **118**, 244303.

- **Y. P. Zhang***, O. Ersoy, A. Karatutlu, W. Little and A. Sapelkin. Local structure of Ge quantum dots determined by combined numerical analysis of EXAFS and XANES data, *J. Synchrotron Rad.*, 2016, **23**, 253-259.

- N. R. C. Corsini, **Y. P. Zhang**, W. R. Little, A. Karatutlu, O. Ersoy, P. D. Haynes, C. Molteni, N. D. M. Hine, I. Hernandez, J. Gonzalez, F. Rodriguez, V. V. Brazhkin and A. Sapelkin*. Pressure-induced amorphization and a new high density amorphous metallic phase in matrix-free Ge nanoparticles, *Nano Lett.*, 2015, **15**, 7334-7340.

- A. Karatutlu*, M. Song, A. P. Wheeler, O. Ersoy, W. R. Little, **Y. P. Zhang**, P. Puech, F. S. Boi, Z. Luklinska and A. V. Sapelkin. Synthesis and structure of free-standing germanium quantum dots and their application in live cell imaging, *RSC Adv.*, 2015, **5**, 20566-20573.

- **Y. P. Zhang***, A. Karatutlu, O. Ersoy, W. Little, G. Cibin, A. Dent, and A. Sapelkin. Structure and effects of annealing in colloidal matrix-free Ge quantum dots, *J. Synchrotron Rad.*, 2015, **22**, 105-112.

- **Y. P. Zhang**, W. Liu and R. Wang*. From ZnS nanoparticles, nanobelts to nanotetrapods: the ethelenediamine modulated anisotropic growth of ZnS nanostructures, *Nanoscale*, 2012, **4**, 2394-2399.

PROJECTS/ASSIGNMENTS (2017–)

Development/Writing/Demonstration/Service:

- Tutorial (for using EXAFS with RMCProfile), maintenance and documentation for RMCProfile & Pipeline setup for continuous integration of RMCProfile.
- Dummy data generation, mixed-phase simulation, local correlation constraint, X-ray total scattering modeling, etc. in RMCProfile.
- Modeling of low-dimensional systems in RMCProfile.
- Correction for resolution effect in RMCProfile.
- Generic implementation of Topas peak profiles in RMCProfile, following a tabulated approach.
- Development of tools for pre-processing of data (e.g. calibration of S(Q) against Bragg) and post-analysis of configurations obtained from RMCProfile (e.g. microstrain & deformation gradient tensor analysis).
- GUI development for RMCProfile.
- Write proposals for the application of beamtime for scattering measurements at various diffractometers (HB2A at HFIR, Oak Ridge; NOMAD at SNS, Oak Ridge and HPCAT at APS, Chicago).
- Demonstration for RMCProfile during 2nd and 3rd total scattering school held at ORNL.
- Communication with users for conducting experiments and data reduction at NOMAD (SNS, Oak Ridge) diffractometer and performing RMCProfile fitting for users' projects & Support visiting PhD students.

Research (ongoing):

- Combination of molecular dynamics simulation and RMCProfile fitting of total scattering data for exploring the structure-property relation in graphitized carbon used as battery anode material.
- Exploration of short-range ordering in cation-disordered oxides for rechargeable lithium batteries through RMCProfile modeling for neutron and X-ray total scattering data.
- Exploration of local magnetic ordering in 2D Van der Vaals magnetic system Fe5-xGeTe2, through RMCProfile modeling of neutron total scattering data.
- Atomistic models of structural relaxations in ceria nanoparticles from neutron total scattering.

Refer to the following sites for relevant resources:
RMCProfile repository on GitLab: https://code.ornl.gov/mth/RMCProfile
RMC tools repository on GitLab: https://code.ornl.gov/zyroc1990/adv_rmc_tools
Personal GitLab for project materials: https://gitlab.com/zyroc1990/iris/tree/master/Research_Projects

CONFERENCES

Oral presentation:

- Y. P. Zhang, Mechanistic Insights into the Superexchange-Interaction-Driven Negative Thermal Expansion in CuO. In: *2019 MRS Fall Meeting and Exhibit*, Boston, US, December 1-6, 2019.
- Y. P. Zhang, Local magnetic cluster size identified by neutron total scattering in the site-diluted spin glass SnxFe4-xN (x=0.88). In: *ACA 2019 Annual Meeting*, Covington, KY, US, July 20-24, 2019.

- Y. P. Zhang, Structural origins of light emission in Ge quantum dots by combination of XAS and optically detected XAS. In: *2017 67th ACA Annual Meeting*, New Orleans, USA, May 26-30, 2017.
- Y. P. Zhang, Structural origins of light emission in Ge quantum dots by combination of XAS and optically detected XAS. In: *PCG Winter Meeting and ISIS Crystallography Users Meeting*, Abingdon, UK, October 19-20, 2015.
- Y. P. Zhang, X-ray Absorption Spectroscopy with other simulation techniques to work on amorphous and nano-systems. In: *2015 E-MRS Fall Meeting*, Warsaw, Poland, September 15-18, 2015.

Poster presentation:

- Y. P. Zhang, Mechanistic Insights into the Superexchange-Interaction-Driven Negative Thermal Expansion in CuO. In: *ACA 2019 Annual Meeting*, Covington, KY, US, July 20-24, 2019.
- Y. P. Zhang, The application of optically-detected X-ray absorption on determining the structural origin of light emission in Ge quantum dots. In: *16 International Conference on X-ray Absorption Fine Structure*, Karsruhe, Germany, August 23-28, 2015.
- Y. P. Zhang, Structure metastability in colloidal matrix-free Ge quantum dots. In: *SR User Meeting 2014*, Diamond Light Source, Oxfordshire, UK, September 13-14, 2014.
- Y. P. Zhang, Structural evolution of matrix-free translucent germanium quantum dots under high pressure. In: *52nd EHPRG meeting*, Lyon, France, September 7-12, 2014.
- Y. P. Zhang, Looking into the structure of Ge nano-crystals through combined Diffraction/EXAFS. In: *The 23rd Congress and General Assembly of the International Union of Crystallography (IUCr 2014)*, Montreal, Canada, August 5-12, 2014.

SKILLS

Research:

- Total scattering (RMCProfile – *PR*, PDFgui – *PR*, Topas – *LP*) • Bragg refinement (GSAS – *PR*, Topas – *PR*) • EXAFS (Demeter – *PR*, FEFF – PR) • XANES (FEFF – *PR*, FDMNES – *PR*, FitIt – *PR*) • Molecular dynamics simulation (DL_POLY – *PR*, LAMMPS – *LP* , GULP – *BE*) • *ab initio* simulation (Quantum Espresso – *FA*, NWCHEM – *BE*).

Programming:

- Fortran *(PR)* • Python (script – *PR*, GUI development with wxpython – *PR*) • Bash script (*FA*) • LaTeX (*FA*) • Makefile (*FA*) • Mathematica (*FA*) • Matlab (including GUI dev, *LE*) • VisualBasic (*LE*) • C (*LE*) • C++ (*BE*) • Parallel programming with OpenMPI (in Fortran, *BE*) • GPU programming with CUDA (*BE*).

Computer skills:

- Graphics processing (Photoshop – *FA*, GIMP – *LP*) • 3D modelling & animation (Blender – *FA*, SketchUp – *LE*).

professional (PR) → less professional (LP) → familiar (FA) → limited experience (LE) → beginner (BE)

AWARDS

• Outstanding Graduate from Beihang University	2012, BEIHANG UNIVERSITY
• Merit Student Prize for the 2009-2010 academic year	2010, BEIHANG UNIVERSITY
• The 3rd-Prize Scholarship of academic performance for the 2009-2010 academic year	2010, BEIHANG UNIVERSITY
• The 3rd-Prize Scholarship of academic performance for the 2008-2009 academic year	2009, BEIHANG UNIVERSITY
• The 2nd-Prize for Physics Contest of Beihang University	2009, BEIHANG UNIVERSITY

OTHER INTEREST/AMATEURS

- Developing little softwares/games. Here is a plane game that I developed using VB: Click Me!

- Diving into the ocean of open source softwares! Here is my desktop configured using the open source tool 'conky' under Ubuntu: Click Me! Here is an animation I produced with open source 3D modeling software Blender, demonstrating the Coriolis force: Click Me!