Final report Ultrafast X-ray spectroscopy on nonequilibrium systems
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What are the major goals of the project?

The goal of the project has been to theoretically investigate a wide variety of problem related to the use of X-ray spectroscopy in materials science to enhance the impact of the science done at DOE's user facilities. The focus has generally been on obtaining a deeper understand of new types of X-ray spectroscopy and to provide support for experimentalist working in these fields. Research topics have included the following.

- Resonant inelastic X-ray scattering. This technique involves the inelastic scattering of X-rays of materials creating excitation inside the material. The scattering process can lead to a wide variety of excitations, such as *dd* transitions, magnons, phonons, charge-density excitations, etc.
- Nonequilibrium X-ray spectroscopy. The advent of pulsed X-ray sources has led to an increase of research of nonequilibrium system using X-ray spectroscopy. Related to this was the need to obtain a better understanding of nonequilibrium processes, such as photoinduced spin-crossover transitions, charge-order melting, and metal-insulator transitions.
- X-ray spectroscopy with X-ray beams carrying orbital angular momentum. In addition to the polarization of the X-rays, beams can be given an orbital moment with the use of special gratings. This leads to unusual spectroscopy and scattering effects.
- Theoretical support of X-ray spectroscopy performed at the Department of Energy's user facilities.

What was accomplished under these goals?

Resonant inelastic X-ray scattering at transition-metal *L* and *M* edges.- In this technique, an incoming X-ray excites an electron from a 2p or 3p core level into the valence shell and one measures the energy of the outgoing X-ray resulting from the recombination of the core hole with a valence electron. Since there is no core hole in the final state, the energy lost by the scattered photon can be related to excitations in the valence shell. This type of RIXS has been used to study *dd* transitions in transition-metal compounds and spin flips and magnon dispersion in high-temperature superconductors and iridates. For RIXS at the transition-metal *L* and *M* edges, the excited electron screens the core-hole potential and valence excitations are mainly created by the radiative transitions. Although the spectral line shape of can often be calculated with numerical methods, the analytical understanding of this provided crucial insights into the potential of these techniques. This proposal laid the foundation for the analytical understanding of RIXS, which led to the use this technique in the study of magnon dispersions. An effective scattering operator approach was used to gain insight into the strength of transitions, such as the elastic peak and spinflip processes. Polarization and angular dependence can be used to selectively probe particular final states.

Resonant inelastic X-ray scattering at transition-metal *K* edges.- This RIXS process studies different types of excitations. Since the 1*s* electron is excited further above the edge, the system predominantly responds to the presence of a strong core-hole potential. The analytical relations between this spectroscopy and the density-density correlation functions have been derived. The dependence of the spectral weights on momentum and various other conditions have been studied in detail. For example, a strong momentum dependence can be observed in manganites.
However, in addition to electronic excitation, the lattice can also respond to the presence of the core hole. This project was at the basis of the theory underlying the excitation of phonons and was involved in the first experimental observation of this effect.

The results of the work on resonant inelastic X-ray scattering were summarized in an article in Review of Modern Physics that has received over 700 citations.

Nonequilibrium phenomena.- The study of nonequilibrium materials using X-ray spectroscopy led to the realization that many of these phenomena were poorly understood. Even in the cases where there was a somewhat better understanding, the work was often done in a theoretical framework unsuitable for the calculation of X-ray absorption and scattering. This required additional research into intersystem crossings, photo-induced metal-insulator transitions and charge-order melting. This work has led to several publications. The major nonequilibrium phenomenon studied was spin crossover, which is summarized below.

Spin crossover complexes.- In a number of transition-metal compounds, the transition metal has two competing spin states, usually characterized as low and high spin. Upon photoexcitation, an electron is transferred to the ligands or between different transition-metal sites. This causes the system to cascade from one spin state to another. The spin flips are enabled by the spin-orbit interaction which does not conserve spin. Additionally, due to the interaction of the electrons on the transition-metal ion a change in the metal-ligand distance is observed. These transitions are very amenable to X-ray spectroscopy and are therefore often used as a model system for nonequilibrium dynamics. Despite the large body of experimental work in both the optical and X-ray region and a decent qualitative understanding of the process, there have been no calculations that describe the time dependence of the process including details such as the full Coulomb multiplet structure, changes in crystal field, and the spin-orbit coupling. All these details are necessary for a successful theoretical description of the time-dependent X-ray spectra in an optical pump/X-ray probe experiment. Successful calculations have been done on spin crossover transition in Fe-Co Prussian blue compounds and for divalent Fe systems. Additionally, the changes in the X-ray spectral line shapes during these transitions have been calculated.

X-ray spectroscopy with orbital-angular momentum carrying beams.- The field of singular optics has grown rapidly after the demonstration that beams with shaped profiles carry orbital angular momentum (OAM). This project has laid the basis for the understanding of the presence of strong dichroic effects induced by x-ray beams carrying orbital angular momentum. Taking the difference between spectra obtained with positive and negative OAM states allows the separation of quadrupolar from dipolar transitions at, e.g., the transition-metal K edges, enabling the study of

the unoccupied states in the absence of strong core-hole effects. The dependence of OAM-induced x-ray dichroism on different polarization vectors was studied and sum rules relating the integrated intensity to ground-state hole densities were derived. Calculations of spectral line shapes for cuprates, manganites, and ruthenates confirm the strong OAM-induced dichroism and indicated the potential of this new spectroscopy in the fields of orbital physics and magnetism.
Additionally, the interaction between two topological objects, an x-ray beam carrying orbital angular momentum and a magnetic vortex, has been studied theoretically. The resonant x-ray scattering intensity was calculated as a function of the relative position of the magnetic and x-ray vortices. For a homogeneous system, the charge scattering is zero. For magnetic scattering, the intensity profile strongly depends on the relative topological indices of the x-ray and magnetic singularities. A strong enhancement in the intensity profile is observed for equal winding factors.

Support for experimental work at DOE's user facilities.- This project has included a wide variety of collaborations with experimentalists from several DOE facilities and users. Additionally, it has involved several international collaborations. Many of the work involved transition-metal compounds. A significant body of work involved cuprates that show high-temperature superconductivity, manganites that exhibit colossal magnetoresistance, and other materials that are known for their unusual magnetic and electronic properties. Recently, a lot of focus has been on iridates, which display interesting spin-orbit physics.

XClaim.- The interpretation of X-ray absorption spectral lineshapes has become relatively standardized for transitions metals and rare-earths. In order to facilitate these calculations for users, a user interface was created for the computer codes that calculate the spectral lineshapes. The codes are available on the website of the Advanced Photon Source at Argonne National Laboratory.

What opportunities for training and professional development has the project provided?

The following postdoctoral associates were supported by the grant

1. Tsezar Seman (2013-2019)
2. Myung-Joon Han (2011-2012, Currently Professor, KAIST, South Korea)
3. Javier Fernández-Rodríguez (2010-2013)
4. Jun Chang (2008-2011. Currently College of Physics and Information Technology, Shaanxi Normal University, Xi'an, China)
5. Eiji Kaneshita (2006-2008. Currently, Professor at Sendai National College of Technology)
6. Serkan Erdin (2004-2006. Currently, Director of Bioinformatics at Massachusetts General Hospital)
7. Ken Ahn (2004-2006. Currently, Professor at New Jersey Institute of Technology)

The following graduate student was supported by the grant

1. William Baker (2018-2020).

How have the results been disseminated to communities of interest?

The results have been published in 73 publications. These include high-impact journals such as Physical Review Letters (17), Scientific Reports (1), Physical Review B Rapid Communications (7), Nature Communications (1), Review of Modern Physics (1) and Science (1). The publication have received over 3300 citations.

Additionally, the work has been presented at numerous conferences.

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What is the impact on the development of the principal discipline(s) of the project?

This project has made a significant impact on the understanding of X-ray spectroscopy. The theoretical basis was laid for several developing and new types of spectroscopy such as resonant inelastic X-ray scattering, X-ray spectroscopy using beams carrying orbital angular momentum, and X-ray spectroscopy on nonequilibrium systems. The work was published in high-impact journals and received as significant number of citations.

What is the impact on other disciplines

Besides considering the impact on X-ray pump probe experiments, the research also sheds light on basic aspects of nonequilibrium dynamical processes, such as spin crossover processes, metal-insulator transitions, and spin and charge-order melting. Although some systems are model systems, the research has helped the understanding dynamical processes in physics and materials science and developing the interpretation of the X-ray spectroscopic tools that measure them. The understanding of nonequilibrium dynamics is relevant for many disciplines, for example, chemical reactions, energy conversion, electronic devices, etc.

Furthermore, the research and the collaboration with experimentalists have made an impact on the field of material science. The materials under consideration are in the field of transition-metal compounds that have (potential) impact in energy storage, ultrafast computing, and high-density memory.

What is the impact on the development of human resources?

The research done in this research has trained researchers for disciplines relevant to the U.S. work force, such as high-performance computing and understanding X-ray science and nonequilibrium dynamics.