Understanding the experiments of the future

Science

In the coming years, research at the Advanced Photon Source will address several of the Grand Challenges listed in the BES report “Directing Matter and Energy – Five Challenges for Science and the Imaginations.” It is expected that X-rays will play a crucial role in understanding these questions. However, experiments in these areas will have substantially less impact or are even impossible to publish without proper theoretical interpretation. The need for theory becomes even more apparent when considering that the challenges involve some of the most complex areas in science, such as strongly correlated multiparticle systems, directed assembly, and matter far beyond equilibrium. A good example of the fruitful interplay between theory and experiment is the work on correlated interfaces where the Theory Group in collaboration with scientists from the Advanced Photon Source, the University of Arkansas, and the Max Planck in Germany found evidence for orbital reconstruction in cuprate-manganite interfaces, Science 318, 1114 (2007). The Theory Group, a joint program between Northern Illinois University and the APS, has been successful in recent years in interacting with experimentalists and providing new initiatives in x-ray science and condensed-matter physics. Its focus is currently on x-ray spectroscopy on strongly correlated materials and magnetism. This base needs to be expanded to address the scientific issues that are and will be addressed by the APS in the future: resonant and nonresonant inelastic x-ray scattering on strongly correlated materials, x-ray spectroscopy of correlated interfaces and nanomaterials, x-ray science under extreme conditions, such as high-pressure, and time-dependent and nonequilbrium spectroscopy. The proposed expansion will significantly enhance the impact of the science done at the APS.

Added value of the medium term upgrade

The Synchron-Related Theory Group requests an increase in manpower to provide theoretical support for the following areas:

- **Time-dependent and nonequilibrium x-ray experiments**. Increasingly, one is using x-rays to study the time-dependent response of materials to an external stimulus, such as a laser pulse or a change in the magnetic field. A successful interpretation of these phenomena could have significant implications for our understanding of photochemistry, photoinduced effects, magnetization dynamics, etc. The interpretation of x-ray experiments on nonequibrium phenomena is only in its initial stages and requires a significant theoretical investment.
- **X-ray absorption and scattering.** These experiments often occur at an absorption edge. The theoretical support for core-level spectroscopy is limited in the U.S. in particular when looking at, e.g. materials under high-pressure, interfacial behavior and nanostructured materials. The need for theory will only increase with the coming on line of the IXS and IEX beamlines, which study density-density correlation functions, high-energy photoemission and orbital/charge ordering in complex materials. In addition, new techniques such as resonant and nonresonant inelastic X-ray scattering or the use of coherence are still not well understood.

- **Structure and dynamics.** There is an extremely wide-range of x-ray techniques used to study and image the structure and dynamics of a broad array of materials ranging from biomaterials, complex disorder, nanostructured materials, self assembly, etc. There are many theoretical and fundamental issues that need to be addressed, such as the use of statistical analysis in materials characterization, the connection between microstructure and macroscopic behavior, the quantitative use of coherence in imaging and dynamics, the relation of scattering data on biomolecules to large-scale motion and eventually function, the relation between complex disorder and macroscopic properties, etc. Whereas it might not be possible to address all these questions, hiring theorists in particular areas could define strong points of research at the APS and make the APS a catalyst for further theoretical research.

The increased strength of the theoretical support will allow the Theory Group to broaden its support for the experimental science done at the APS, and, in addition, to perform more fundamental research that help define future experimental directions, provide the underlying framework for experiments, and set out new pathways to increase the amount of information that can be extracted from experiments.

Expected user communities

The requested expansion of the Theory Group will significantly expand the scope of the research done allowing the Theory Group to address several areas in x-ray spectroscopy and scattering, directed assembly, nonequilbrium phenomena, etc. The requested money to establish a Visitor Institute will enable the Theory Group to invite theorists or support beamlines that want to invite visitors for shorter or longer periods. The Theory Group will interact with user and beamline scientists of the XOR beamlines. Interaction with users will occur in a collaborative fashion, where users directly contact the Theory Group or with beamline scientists acting as an intermediary. The advantages of having a strong in-house theory group is that experimentalists can directly communicate with theorists that are experts in their field and in experiments performed using X-rays who can help with the interpretation of experiments or aid in establishing connections. The Theory Group can also guide in the development of scientific software and simulation tools at the APS.

Enabling technology and infrastructure

The theory will involve a wide range of theoretical techniques, such as Density Functional Theory, many-body calculations, Monte-Carlo type calculations, molecular dynamics, and analytical calculations. The group will make use of personal computers and existing computational facilities at Argonne. The Theory Group will also interact with theorists at the Materials Science Division, the Chemistry Division, the Center for Nanoscale Materials, and Mathematics and Computer Science.

In addition, the group will coordinate its efforts with the Scientific Software Group. Codes being developed in the Theory Group that will be of use to the community, will be incorporated into the platforms developed by the Scientific Software group.

Partnership and user interest

John Hill, Scientist, Brookhaven National Laboratory.
Thomas Gog, Scientist, Advanced Photon Source.
Peter Abbamonte, Professor of Physics, University of Illinois, Urbana-Champaign
Juan-Carlos Campuzano, Professor of Physics, University of Illinois, Chicago
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Jacques Chakhalian, Professor of Physics, University of Arkansas.
Lin Chen, Chemistry Division, Argonne National Laboratory.
Daniel Haskel, Advanced Photon Source.
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Industry and technology transfer

None foreseen at the moment.

Estimated budget

The budget involves a visitors institute, allowing to attract several short and longer term visitors each year that will stimulate the science at the Advanced Photon Source. A request is made for an increase in staff of three permanent staff members essential to provide theoretical support for the new science directions that will be initiated by the APS. Additional postdoctoral in also included.

	Year 1	*Year 2*	*Year 3*	*Year 4*	*Year 5*	*Total*
Visitors	20	30	40	40	50	180
Staff	0	200	200	400	600	1400
postdoc	0	90	90	180	180	540
total	20	320	330	620	830	2130

amounts in k$.