

Final Technical Report

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Lead Institution: Northeastern University, Boston

Title: *Building a Unified Computational Model for the Resonant X-Ray Scattering of Strongly Correlated Materials*

Principal Investigators: A. Bansil (Lead-PI), J.K. Freericks (co-PI), M. van Veenendaal (co-PI)

Basic-Energy Sciences of the Department of Energy (BES/DOE) has made large investments in x-ray sources in the U.S. (NSLS-II, LCLS, NGLS, ALS, APS) as powerful enabling tools for opening up unprecedented new opportunities for exploring properties of matter at various length and time scales. The coming online of the pulsed photon source, literally allows us to see and follow the dynamics of processes in materials at their natural timescales. There is an urgent need therefore to develop theoretical methodologies and computational models for understanding how x-rays interact with matter and the related spectroscopies of materials.

The present project addressed aspects of this grand challenge of x-ray science. In particular, our Collaborative Research Team (CRT) focused on understanding and modeling of elastic and inelastic resonant X-ray scattering processes. We worked to unify the three different computational approaches currently used for modeling X-ray scattering—density functional theory, dynamical mean-field theory, and small-cluster exact diagonalization—to achieve a more realistic material-specific picture of the interaction between X-rays and complex matter. To achieve a convergence in the interpretation and to maximize complementary aspects of different theoretical methods, we concentrated on the cuprates, where most experiments have been performed. Our team included both US and international researchers and it fostered new collaborations between researchers currently working with different approaches. In addition, we developed close relationships with experimental groups working in the area at various synchrotron facilities in the US. Our CRT thus helped toward enabling the US to assume a leadership role in the theoretical development of the field, and to create a global network and community of scholars dedicated to X-ray scattering research.

The CMCSN funding provided the ‘glue’ funding without which the collaborative research activities that were undertaken under this award would not have been possible. The CMCSN funding was thus a critically important enabler in this connection. The collaborative activities started under the CMCSN award led to further collaborative work within the team members even after the CMCSN funding ended.

Details of the research accomplished under this award are presented in the list of publications in open, peer-reviewed literature given below.

In short, we were able to accomplish the goals of our CMCSN project extremely well.

List of CMCSN-supported Publications

1. K. H. Ahn, A.J. Fedro, and Michel van Veenendaal, "Dynamics and spectral weights of shake-up valence excitations in transition metal K-edge resonant inelastic x-ray scattering", *Phys. Rev. B.* 79, 045103 (2009).
2. Luuk J. P. Ament, Giacomo Ghiringhelli, Marco Moretti Sala, Lucio Braicovich, and Jeroen van den Brink, "Theoretical Demonstration of How the Dispersion of Magnetic Excitations in Cuprate Compounds can be Determined Using Resonant Inelastic X-Ray Scattering", *Phys. Rev. Lett.* 103, 117003 (2009).
3. B. Moritz, T. P. Devereaux, and J. K. Freericks, "Time-resolved photoemission of strongly correlated electrons driven out of equilibrium", *Phys. Rev. B* 81, 165112 (2010).
4. L. Braicovich, M. Moretti Sala, L. J. P. Ament, V. Bisogni, M. Minola, G. Balestrino, D. Di Castro, G. M. De Luca, M. Salluzzo, G. Ghiringhelli, and J. van den Brink, "Momentum and polarization dependence of single-magnon spectral weight for Cu L3-edge resonant inelastic x-ray scattering from layered cuprates", *Phys. Rev. B* 81, 174533 (2010).
5. O. P. Matveev, A. M. Shvaika, and J. K. Freericks, "Nonresonant Raman and inelastic X-ray scattering in the charge-density-wave phase of the spinless Falicov-Kimball model", *Phys. Rev. B* 79, 115130 (2009).
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10. H. Yavas, M. van Veenendaal, J. van den Brink, L.J.P. Ament, A. Alatas, B.M. Leu, M.-O. Apostu, Nadia Wizen, Gunter Behr, W. Sturhahn, E.E. Alp, and Harald Sinn,

- “Observation of phonons with resonant inelastic x-ray scattering”, *J. Phys.: Condens. Matter* **22**, 485601 (2010).
11. C.-C. Chen, B. Moritz, C. J. Jia, S. Johnston, A. P. Sorini, L.-Q. Lee, K. Ko, and T. P. Devereaux, “Numerical studies of photon- based spectroscopies on high-Tc superconductors,” *Computer Physics Communications* **182**, 106-108 (2011)
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