

Wei Ku

Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, Bldg 510
Upton, NY 11973-5000

(631) 344-2684

weiku@bnl.gov / weiku@mailaps.org

<http://www.cmth.bnl.gov/~weiku/>

-
- Education**
- 1995-2000 **University of Tennessee** Knoxville, TN
Ph.D. Physics -- Thesis "Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Particle Systems"
- 1994-1995 **Georgia State University** Atlanta, GA
15 credit-hours of course work
- 1987-1991 **Tamkang University** Tamsui, Taiwan ROC
B.S. Physics
- Honors**
- Lawrence Fellowship in Lawrence Livermore National Lab (2003) (fellowship declined)
Joe Fowler & Jerry Marion Outstanding Graduate Student Award in Department of Physics, University of Tennessee, Knoxville, USA (1998)
Department Head's Award in Department of Physics, TamKang University, Tamsui, Taiwan ROC (1988)
- Activities**
- American Physical Society (1999-Present)
Vice president of Chinese Student Association at the University of Tennessee, Knoxville (1997)
UT/ORNL Collaborative Scientist Program (1996-2000)
- Skills**
- All-electron based first-principles many-body theory of condensed matter systems
Quantum magnetism of strongly correlated systems, based on *ab initio* Wannier function analysis
Dynamical charge/magnetic response within time-dependent density functional theory
Quasi-particle excitation spectrum within finite temperature many-body perturbation theory
Quantum Monte Carlo method
Parallel scientific computing (MPI, and OpenMP)
Object-oriented numerical methods
Computer programming: C++, C, FORTRAN, BASIC, and assembly
Platform operation: IBM SP, PC Cluster (with DOS, Windows, or LINUX), Sun Sparc, DEC Alpha, IBM RS6000, and Cray T3E
- Relevant Experience**
- 2005-present **Brookhaven National Laboratory** Upton, NY
Associate Physicist
- 2003-present **Stony Brook University** Stony Brook, NY
Adjunct Professor
- 2003-2005 **Brookhaven National Laboratory** Upton, NY
Associate Physicist
- First-principles derivation of effective reduced Hamiltonian via numerical CD renormalization group methods
Bi-orthogonal interpolating wavelet based $O(N)$ energy minimization approach to density functional theory
Missing Fermi pockets and Fermi-topology of Na_xCoO_2
Thermal fluctuation of phase of superconducting order parameter
Microscopic electron and phonon mechanisms of charge density wave and charge order
Material dependence of high- T_c cuprates
Microscopic mechanisms of orbital/charge order of manganites
Gapless charge density wave in transition metal dichalcogenides

- Local excitations of Mott insulators and charge transfer insulators
Hybridization and propagation of local Frenkel excitons
- 2001-2003 **University of California** Davis, CA
Post-graduate Researcher
- Multi-energy-resolution construction of all-electron Wannier functions of highly correlated systems
Microscopic analysis of magnetic structure of spin-Peierls CuGeO_3 , spin-spiral CuSiO_3 , and ferromagnetic Li_2CuO_2 chains
Dynamical density response of transition metals and oxides (LDA+U)
Pressure dependence of ferromagnetism of semiconducting EuO, EuS, EuSe, and EuT
Insulating ferromagnetism in half-filled $\text{La}_4\text{Ba}_2\text{Cu}_2\text{O}_{10}$
Microscopic origin of complex magnetic structure of $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$
Ab initio construction of 2^{nd} -quantized lattice Hamiltonian using all-electron Wannier functions
Construction of energy-resolved all-electron Wannier function
2D Hubbard model (Quantum Monte Carlo) study of stripes in doped High-Tc superconductors
Collective charge excitations in MgB_2
- 1997-2000 **University of Tennessee** Knoxville, TN and **Solid State Division, ORNL** Oak Ridge, TN
Graduate Research Assistant
- Thesis “Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Particle Systems”: first-principles study of electronic excitations in realistic condensed matter within two theoretical frameworks: time-dependent density functional theory (TDDFT), for study of linear density response, and finite-temperature many-body perturbation theory (MBPT) with Kadanoff-Baym conserving (self-consistent) scheme, for study of quasi-particle excitation. Systems studied include simple metals, transition metals and semiconductors.
- Quasi-particle excitation spectrum of proto-type semiconductors, Si and Ge
Many-body self-consistency effect on quasi-particle bandwidth of Na
Pure Matsubara time, all-electron, self-consistent *GW* implementation of finite-temperature many-body perturbation theory
d-threshold charge response of Zn and Cd
Absence of Landau damping in Cs
Anomalous plasmon lifetime dispersion of K
All-electron, LAPW implementation of TDDFT linear density response
Proposal, design, construction, and configuration of Linux PC cluster “Hive” in the Solid State Division for parallel computing.
- 1995-1996 **University of Tennessee** Knoxville, TN
Graduate Teaching Assistant
- Undergraduate Lab teaching
- 1994-1995 **Georgia State University** Atlanta, GA
Graduate Teaching Assistant
- Undergraduate Lab teaching
- 1993-1994 **Tamkang University** Tamsui, Taiwan, ROC
Coordinator of General Physics Lab.
- Equipment setup and maintenance for General Physics Lab
Experiment design and improvement
Graduate teaching assistants training and qualifying

- Representative Publications**
- “Dynamical reconstruction of the exciton in LiF with inelastic x-ray scattering”
Peter Abbamonte, Tim Graber, James P. Reed, Serban Smadici, Chen-Lin Yeh, Abhay Shukla, Jean-Pascal Rueff, and Wei Ku, submitted to PNAS (2008)
 - “Hybridization of local Frenkel excitons in strongly correlated NiO: a first-principles Wannier function approach”
Chi-Cheng Lee, Hung-Chung Lee, and Wei Ku, in preparation

- “Charge Ordering in Half-Doped Manganites: Weak Charge Disproportion and Leading Mechanisms”
D. Volja, W.-G. Yin, and Wei Ku, submitted to Phys. Rev. Lett. (2007)
- “Tuning Hole Mobility, Concentration, and Repulsion in High-Tc Cuprates via Apical Atoms”
W.-G. Yin and Wei Ku, submitted to Phys. Rev. Lett. (2007)
- “Nanoscale Disorder in $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$: A New Route to the Enhanced Dielectric Response”
Y. Zhu, J. C. Zheng, L. Wu, A. I. Frenkel, J. Hanson, P. Northrup, and W. Ku, Phys. Rev. Lett. **99**, 037602 (2007)
- “Non-resonant Inelastic X-Ray Scattering and Energy-Resolved Wannier Function Investigation of $d-d$ Excitations in NiO and CoO”
B. C. Larson, Wei Ku, J. Z. Tischler, Chi-Cheng Lee, O. D. Restrepo, A. G. Eguiluz, P. Zschack, and K. D. Finkelstein, Phys. Rev. Lett. **99**, 026401 (2007)
- “Low-Energy Charge-Density Excitations in MgB_2 : Striking Interplay between Single-Particle and Collective Behavior for Large Momenta”
Y. Q. Cai *et al.*, Phys. Rev. Lett. **97**, 176402 (2006)
- “Orbital ordering in LaMnO_3 : Electron-lattice versus electron-electron interactions”
W.-G. Yin, D. Volja, and Wei Ku, Phys. Rev. Lett. **96**, 116405 (2006)
- “Coexistence of gapless excitations and commensurate charge-density wave in the 2H-transition metal dichalcogenides”
R. L. Barnett, A. P., E. Demler, W.-G. Yin, and Wei Ku, Phys. Rev. Lett. **96**, 026406 (2006)
- “ $d-d$ Excitations in Manganites Probed by Resonant Inelastic X-Ray Scattering”
S. Grenier, J. P. Hill, Wei Ku, V. Kiryukhin, V. Oudovenko, Y.-J. Kim, K. J. Thomas, S.-W. Cheong, Y. Tokura, Y. Tomioka, D. Casa, and T. Gog, Phys. Rev. Lett. **94**, 047203 (2005)
- “Insulating Ferromagnetism in $\text{La}_4\text{Ba}_2\text{Cu}_2\text{O}_{10}$: an *Ab Initio* Wannier Function Analysis”
Wei Ku, H. Rosner, W. E. Pickett, and R. T. Scalettar, Phys. Rev. Lett. **89**, 167204 (2002)
- “Band-Gap Problem in Semiconductors Revisited: Effects of Core States and Many-Body Self-Consistency”
Wei Ku and A. G. Eguiluz, Phys. Rev. Lett. **89**, 126401 (2002)
- “*Ab Initio* Investigation of Collective Charge Excitations in MgB_2 ”
Wei Ku, W. E. Pickett, R. T. Scalettar, and A. G. Eguiluz, Phys. Rev. Lett. **88**, 057001 (2002)
- “Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Particle Systems”
Wei Ku, thesis, University of Tennessee, Knoxville (2000)
- “Comment on ‘Why is the bandwidth of sodium observed to be narrower in photoemission experiments?’ ”
Wei Ku, A. G. Eguiluz, and W. E. Plummer, Phys. Rev. Lett. **85**, 2410 (2000)
- “Plasmon Lifetime in K: A Case Study of Correlated Electrons in Solids Amenable to *Ab Initio* Theory”
Wei Ku and A. G. Eguiluz, Phys. Rev. Lett. **82**, 2350 (1999)
- “Crucial Role of the Crystal Potential in Magnetism of Edge-Sharing Cu-O Chains and its Interplay with the Bond Angle”
H. Rosner, Wei Ku, R. T. Scalettar, W. E. Pickett, S.-L. Drechsler, J. Malek, R. Neudert, M. Knupfer, J. Fink, and H. Eschrig, unpublished

**Other
Publications**

- “A Novel First-Principles Approach to Effective Hamiltonians for high-Tc superconducting cuprates”
Wei-Guo Yin and Wei Ku, submitted to JPCS (conference proceedings of LEHTSC2007).
- “Synthesis of Ultrathin Palladium and Platinum Nanowires and a Study of Their Magnetic Properties”
Xiaowei Teng, Wei-Qiang Han, Wei Ku, Markus Hücker, *Angewandte Chemie International Edition*, **47**, 2055 (2008).
- “Effect of Number of Walls on Plasmon Behavior in Carbon Nanotubes”
M. H. Upton, R. F. Klie, J. P. Hill, T. Gog, D. Casa, W. Ku, Y. Zhu, M. Y. Sfeir, J. Misewich, G. Eres, D. Lowndes, submitted to *Phys. Rev. B* (2006)
- “Universal quasiparticle decoherence in hole- and electron-doped high-Tc cuprates”
Z.-H. Pan, P. Richard, A.V. Fedorov, T. Kondo, T. Takeuchi, S.L. Li, Pengcheng Dai, G.D. Gu, W. Ku, Z. Wang, and H. Ding, submitted to *Phys. Rev. Lett.* (2006)
- “Nature of oxygen dopant-induced states in high-temperature Bi₂Sr₂CaCu₂O_{8+x} superconductors: A photoemission investigation”
P. Richard, Z.-H. Pan, M. Neupane, A. V. Fedorov, T. Valla, P. D. Johnson, G. D. Gu, W. Ku, Z. Wang, and H. Ding, *Phys. Rev. B* **74**, 094512 (2006)
- “Unusual photoemission resonances of oxygen-dopant induced states in Bi₂Sr₂CaCu₂O_{8+δ}”
P. Richard, Z.-H. Pan, M. Neupane, A. V. Fedorov, T. Valla, P. D. Johnson, G. D. Gu, W. Ku, Z. Wang, and H. Ding, (preprint)
- “Electron-hole and plasmon excitations in 3d transition metals: Ab initio calculations and inelastic x-ray scattering measurements”
I. G. Gurtubay, J. M. Pitarke, Wei Ku, A. G. Eguiluz, B. C. Larson, J. Tischler, P. Zschack, and K. D. Finkelstein, *Phys. Rev. B* **72**, 125117 (2005)
- “Exchange Coupling in Eu Monochalcogenides from First Principles”
J. Kunes, Wei Ku, and W. E. Pickett, *J. Phy. Soc. Jap.*, **74**, 1408 (2005)
- “Comment on “Band-Gap problem in semiconductors revisited: Effects of core states and many-body self-consistency” – Reply”
Wei Ku, A. G. Eguiluz, *Phys. Lett.* **93**, 249702 (2004)
- “Large crystal local-field effects in the dynamical structure factor of rutile TiO₂”
I. G. Gurtubay, Wei Ku, J. M. Pitarke, A. G. Eguiluz, B. C. Larson, J. Tischler, and P. Zschack, *Phys. Rev. B* **70**, 201201 (2004)
- “Effects of the crystal structure in the dynamical electron-density response of hcp transition metals”
I. G. Gurtubay, Wei Ku, J. M. Pitarke, and A. G. Eguiluz
Computational Materials Science **30**, 104 (2004)
Selected papers of the Twelfth International Workshop on Computational Materials Science (CMS2002)
- “Microscopic analysis of Insulating Magnetism of La₄Ba₄Cu₂O₁₀ and Nd₄Ba₄Cu₂O₁₀”
Wei Ku, H. Rosner, W. E. Pickett, and R. T. Scalettar, *J. Solid State Chem.* **171**, 329 (2003)
- “Self-interaction correction and contact hyperfine field”
P. Novák, J. Kune, W. E. Pickett, Wei Ku, and F. R. Wagner, *Phys. Rev. B* **67**, 140403 (2003)
- “PAR-dependent and geometry-dependent mechanisms of spindle positioning”
M.-F. B. Tsou, Wei Ku, A. Hayashi, and L. S. Rose, *J. Cell Bio.* **160**, 845 (2003)
- “MgB₂: Complex Behavior from a Simple Compound”
H. Rosner, J.M. An, W. Ku, M.D. Johannes, R.T. Scalettar, W.E. Pickett, S.V. Schulga, S.-L. Drechsler, H. Eschrig, W. Weber, and A.G. Eguiluz, *Studies of High Temperature Superconductors*, Vol. **38**, edited by A. Narlikar (Nova, New York, 2001)
- “Dynamical Response of Correlated Electrons in Solids Probed by Inelastic Scattering Experiments: An *Ab Initio* Theoretical Perspective”
A. G. Eguiluz, Wei Ku and J. M. Sullivan, *J. Phys. Chem. Solids* **61**, 383 (2000)
- “*Ab Initio* Studies of Electronic Excitations in Real Solids”
Adolfo G. Eguiluz and Wei Ku, *Electron Correlations and Materials Properties*, edited by A. Gonis, N. Kioussis, and M. Ciftan (Kluwer Academic, New York, 1999), p. 329
- “Anomalous Loss Functions of Zn and Cd: Dynamical *d*-Threshold and Coherent Electron-Hole Response”
Wei Ku, and Adolfo G. Eguiluz, unpublished

**Invited
Presentations**

- “Tuning in-plane behavior of high- T_c cuprates via apical atoms: New theoretical findings on the material dependence”
Sanibel Symposium (St. Simons Island, Georgia, February 2008)
- “Utilizing the short wavelength of X0-ray to study low-energy local excitations: q-dependence of the spectral weights and dispersions”
Workshop on “Inelastic X-ray Scattering at NSLS-II” (NSLS-II, January 2008)
- “Recent First-Principles Studies of Strongly Correlated Systems: Gapless CDW, orbital/charge ordering and superconducting pair suppression”
International workshop on “Novel Methods for Electronic Structure Calculations” (La Plata, Argentina, November 2007)
- “Tuning in-plane behavior of high- T_c cuprates via apical atoms: New theoretical findings on the material dependence”
LEHTSC2007 “International Symposium on Lattice Effects in Cuprate High Temperature Superconductors – Spin, phonon or third way?” (Tsukuba, Japan, October 2007)
- “Recent First-Principles Studies of Strongly Correlated Systems: Gapless CDW, orbital/charge ordering and superconducting pair suppression”
Physics Department, University of California, Davis (Davis, September 2007)
- “Local excitations in strongly correlated multi-orbital systems: effective kinetic effects in one-and two-particle channels”
CMSN workshop (Davis, September 2007)
- “Recent First-Principles Studies of Strongly Correlated Systems: Gapless CDW, orbital/charge ordering and superconducting pair suppression”
“Wannier functions: what you can do with it and how”
Max-Planck Institute for Chemical Physics of Solids (Dresden, July 2007)
- “Finite-temperature many-body perturbation theory and conserving scheme”
“Wannier functions: what you can do with it and how”
Department of Materials Physics, University of Leoben (Leoben, July 2007)
- “Recent First-Principles Studies of Strongly Correlated Systems: Gapless CDW, orbital/charge ordering and superconducting pair suppression”
Department of Magnetism and Superconductivity Institute of Physics (Prague, July 2007)
- “Recent First-Principles Studies of Strongly Correlated Systems: Gapless CDW, orbital/charge ordering and superconducting pair suppression”
Department of Physics, University of Nurnberg-Erlangen (Erlangen, July 2007)
- “Recent First-Principles Studies of Strongly Correlated Systems: Gapless CDW, orbital/charge ordering and superconducting pair suppression”
Center for Electronic Correlations and Magnetism Theoretical Physics III, University of Augsburg (Augsburg, June 2007)
- “Symmetry Respecting Wannier Functions and Their Applications in Strongly Correlated Systems: New Development of First-Principles Many-Body Down-Folding Approach”
CECAM workshop “Maximally Localized Wannier Functions: Concepts, Applications, and Beyond” (Lyon, June 2007)
- “Recent First-Principles Studies of Strongly Correlated Systems: Gapless CDW, orbital/charge ordering and superconducting pair suppression”
CNRS - Institut Néel (Grenoble, June 2007)
- “Tuning Hold Mobility, Concentration, and Repulsion in High- T_c Cuprates via Apical Atoms: new theoretical findings on the material dependence”
DFLFS3 (Port Jefferson, May 2007)
- “Tuning Hold Mobility, Concentration, and Repulsion in High- T_c Cuprates via Apical Atoms”
CMSN workshop (Denvor, March 2007)
- “Recent First-Principles Studies of Strongly Correlated Systems: Gapless CDW, orbital/charge ordering and others”
LLNL international workshop on “Correlated Electrons in Matter” (Half Moon Bay, December 2006)
- “Recent First-Principles Studies of Strongly Correlated Systems: Gapless CDW, orbital/charge ordering

and others”

NRL (Washington DC, November 2006)

- “Recent First-Principles Studies of Strongly Correlated Systems: Material dependence of high-T_c cuprates”
Academia Sinica (Taipei, June 2006)
- “Recent first-principles studies of strongly correlated systems: gapless CDW, orbital ordering and others”
Department of Physics, TKU (Tamsui, June 2006)
- “Bridging first-principles methods and many-body models”
OPCA5 (Taipei, Taiwan, Jun 2006)
- “First-Principles Many-Body Theories of Excitation and Strongly Correlated Systems”
special summer school, NCKU (Tainan, ROC, Jun 2006)
- “Filling the missing pieces of the puzzles in strongly correlated systems”
Department of Physics, UIUC (Urbana, June 2006)
- “Probing local excitations with angular dependence of large-q non-resonant IXS: Sensitivity to weak electronic symmetry breaking in NiO and CoO”
APS user meeting, ANL (Chicago, May 2006)
- “Recent development of Wannier function and its applications to electronic excitations in strongly correlated systems”
workshop on “First-principles approaches to optical and photoelectron spectra” (Munich, March 2006)
(declined due to US visa related issues)
- “First-Principles Study of Strongly Correlated Systems: filling the missing pieces of the puzzles”
Department of Physics, Boston College (Boston, November, 2005)
- “Applications of Wannier Functions and Derivation of Effective Hamiltonian of Strongly Correlated Systems”
CMSN workshop (Chicago, September 2005)
- “First-Principles Study of Strongly Correlated Systems: filling the missing pieces of the puzzles”
Department of Physics, Pennsylvania State University (November, 2005)
- “First-Principles Study of Strongly Correlated Systems: filling the missing pieces of the puzzles”
Department of Physics, Harvard University (Boston, June, 2005)
- “First-Principles Study of Strongly Correlated Systems: filling the missing pieces of the puzzles”
Department of Physics, Columbia University (New York, April, 2005)
- “First-Principles Study of Strongly Correlated Systems: filling the missing pieces of the puzzles”
Department of Physics, University of California at Irvine (Irvine, February, 2005)
- “Energy-Resolved Wannier States with Assigned Local Symmetry : Recent Development & Applications”
CMSN workshop, (Oak Ridge, September 2004)
- “Textbook Perturbation Theory at Work in Real Semiconductors: What's all the recent arguments on GW calculations about?”
Department of Physics, Rutgers University (Piscataway, April 2003)
- “First-Principles Methods of Quasi-Particle and Electron-Hole Excitations”
International Workshop on Computational Materials Physics (Taipei, Taiwan, November 2003)
- “Magnetic Coupling in Insulating Quasi-1D Cu-O Spin Chains: Toward Fully First-Principles Approaches for Strong Correlation”
Workshop on Advanced Material Science (Tamsui, Taiwan, November 2003)
- “First-Principles Methods of Quasi-Particle and Electron-Hole Excitations”
Department of Physics, Tamkang University (Tamsui, Taiwan, November 2003)
- “Magnetic Coupling in Insulating Quasi-1D Cu-O Spin Chains: Toward Fully First-Principles Approaches for Strong Correlation”
National Center of Theoretical Sciences (Hsinchu, Taiwan, November 2003)
- “Magnetic Coupling in Insulating Quasi-1D Cu-O Spin Chains: Toward Fully First-Principles Approaches for Strong Correlation”
Department of Physics, National Sun Yat-Sen University (Kaohsiung, Taiwan, November 2003)

- “Simple Construction of Energy-Resolved Wannier States with Assigned Local Symmetry”
CMSN workshop (Knoxville, November 2003)
- “Magnetic Coupling in Insulating Quasi-1D Cu-O Spin Chains: Toward Fully First-Principles Approaches for Strong Correlation”
Department of Physics, SUNY Stony Brook (Stony Brook, October 2003)
- “Quasi-Particle Excitation in Semiconductors: All-Electron Conserving *GW* scheme”
ES2003 - Fifteenth Annual Workshop on Recent Developments in Electronic Structure Methods (Minneapolis, May 2003)
- “New Understanding and Surprises from Novel Realistic Many-Body Methods: Quasi-Particle Spectrum of Semiconductors and Insulating Ferromagnetism in Cuprates”
Lawrence Berkeley National Lab (April, 2003)
- “Wannier Function Study of Insulating Ferromagnetism”
APS March Meeting (Austin, March 2003)
- “Dynamical Electronic Excitations in Real Materials: Perspective of First-Principles Many-Body Theories”
McGill University (Montreal, February 2003)
- “Dynamical Electronic Excitations in Real Materials: Perspective of First-Principles Many-Body Theories”
Lawrence Livermore National Laboratory (Livermore, February 2003)
- “Dynamical Electronic Excitations in Real Materials: Perspective of First-Principles Many-Body Theories”
Brookhaven National Lab (Upton, November 2002)
- “Wannier State Analysis of Insulating Ferromagnetism in $\text{La}_4\text{Ba}_2\text{Cu}_2\text{O}_{10}$ ”
ESCM - Electronic Structure and Computational Magnetism (Washington DC, July 2002)
- “Wannier State Analysis of Insulating Ferromagnetism in $\text{La}_4\text{Ba}_2\text{Cu}_2\text{O}_{10}$ ”
Department of Physics, USC (LA, June 2002)
- “Microscopic Analysis of Non-Metallic Ferromagnetism in $\text{La}_4\text{Ba}_2\text{Cu}_2\text{O}_{10}$ Based on *Ab Initio* Wannier Functions”
Department of Physics, UC Davis (Davis, March 2002)
- “Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Body systems”
Material Research Institute, Lawrence Livermore National Laboratory (Livermore, May 2001)
- “Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Body systems”
Department of Physics, UC Davis (Davis, September 2000)
- “Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Body systems”
Solid State Division, Oak Ridge National Laboratory (Oak Ridge, September 2000)
- “Non-uniform Time Axis Technique and All-electron Self-consistent GWA for Si band gap”
CECAM - Excited states and electronic spectra (Lyon, July 2000)
- “First Principle Study of Electronic Excitation in Condensed Matter: A Bridge Connecting Experiment and Physical Picture”
Department of Physics, UT Knoxville (Knoxville, April 2000)
- “Collective Modes in Simple Metals: Plasmon, Zone Boundary Collective State, and Core Dipole Collective Mode”
Department of Physics, UT Knoxville (Knoxville, September 1998)
- “Functional minimization scheme for first-principles electronic structure calculations with bi-orthogonal interpolating wavelets”
“Layer Dependence of Charge Distribution and Electronic Structure of $\text{HgBa}_2\text{Ca}_4\text{Cu}_5\text{O}_{12}$ ”
“Tuning Hole Mobility, Distribution and Repulsion in High-Tc Cuprates via Apical Atoms”
“Phonon Softening and Displacement Pattern in Commensurate Charge Density Wave in 2H-TaSe_2 ”
“Phase Fluctuations in high-Tc Superconductors”
“Strong hybridization of Frenkel excitons in Mott insulators: a novel Wannier function perspective”

**Presentations/
Conferences**

- “Propagation of strongly bound Frenkel excitons in LiF: An effective two-particle kinematic approach of super-atom in ab initio Wannier basis”
- “Investigation of Dipole-Forbidden d-d Excitations in Strongly Correlated Transition-Metal Oxides Using Higher-Order Multipole, Non-resonant Inelastic X-Ray Scattering”
- “Charge Ordering in Half-Doped Manganites: Small Charge Disproportion and Leading Mechanisms”
- “Dynamical reconstruction of the valence exciton in LiF”
- APS March Meeting (New Orleans, March 2008)
- “Tuning Hole Mobility, Concentration, and Repulsion in High- T_c Cuprates via Apical Atoms”
BNL (Upton, May 2007)
 - “Hybridization of Local Frenkel Excitons in NiO”
“Inelastic X-ray Scattering Studies of Plasmons in Carbon Nanotubes”
“Non-Resonant Inelastic X-Ray Scattering and Energy-Resolved Wannier Function Investigation of $d-d$ Excitations in NiO and CoO”
“Tuning effective interactions in high- T_c cuprates via apical oxygen atoms: New realization from the first-principles Wannier function approach”
“Weak charge disproportion and leading mechanisms in half-doped manganites”
APS March Meeting (Denver, March 2007)
 - “Symmetry broken states of interacting particles in condensed matter systems”
Department of Physics, SUNY-Stony Brook (Stony Brook, October 2006)
 - “Electronic Symmetry Breaking Probed via Local In-Gap Excitations in NiO and CoO: Application of First-Principles Wannier Functions to Linear Response of Strongly Correlated Systems”
International workshop on “Density functional theory meets strong correlation”, poster (Montauk, September 2006)
 - “Lattice, Charge, Magnetic and Orbital Ordering of insulating $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ ”
International workshop on “Density functional theory meets strong correlation”, poster (Montauk, September 2006)
 - “Material dependence of high- T_c cuprates: recent theoretical findings”
BNL (Upton, May 2006)
 - “Non-resonant Inelastic X-Ray Scattering and Energy-Resolved Wannier Function Investigation of Local Excitations in NiO and CoO”
“First-Principles Construction of the Zhang-Rice singlet: Role of the apical oxygen in the mobility of the doped hole”
“Theoretical study of charge, spin, and orbital order in half-doped $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ ”
“A realistic approach to effective Hamiltonians for strongly correlated electron materials: Study of orbital ordering in LaMnO_3 ”
“Non-resonant Inelastic X-Ray Scattering and Energy-Resolved Wannier Function Investigation of Local Excitations in Transition Metal Monoxides NiO and CoO”
APS March Meeting (Baltimore, March 2006)
 - “Broken Symmetry in Condensed Matter Systems”
Department of Physics, SUNY Stony Brook University (Stony Brook, October 2005)
 - “Gapless charge density wave in (triangular lattice) 2H-transition metal dichalcogenides”
Brookhaven National Lab (Upton, October 2005)
 - “Lattice, Charge, Magnetic and Orbital Ordering of insulating $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ ”
“A First-Principles Approach to Effective Hamiltonians for Strongly Correlated Electron Materials: Electronic Symmetry Breaking Probed via Local In-Gap Excitations in NiO and CoO: Application of First-Principles Wannier Functions to Linear Response of Strongly Correlated Systems”
ES2005 - Annual Workshop on Recent Developments in Electronic Structure Methods (Cornell, June 2005) (poster)
 - “Pseudo-Spin of Orbital-Ordered Hybridized eg -States in Manganites”
“Theoretical Study of Orbital and Lattice Structure of MnF_3 : the origin of orbital ordering”
“Electron interaction effects on Jahn-Teller instability in LaMnO_3 ”
“The Dynamical Structure Factor of NiO and CoO”
APS March Meeting (Las Angeles, March 2005)

- CFN Users' Meeting, Brookhaven National Lab (Upton, May 2004)
- “Theoretical Study of Magnetic, Orbital and Lattice Structure of MnF₃: Is Jahn-Teller Distortion Necessary for Orbital Ordering?”
ES2004 - Annual Workshop on Recent Developments in Electronic Structure Methods (Rutgers, June 2004) (poster)
- “Theoretical Study of Magnetic, Orbital and Lattice Structure of MnF₃: Is Jahn-Teller Distortion Necessary for Orbital Ordering?”
NSLS annual users' meeting, BNL (Upton, May 2004) (poster)
- “Origin of Magnetic Coupling in Quasi-1D Edge-Sharing Cu-O Chains: Role of the Crystal Potential”
Department of Physics, BNL (Upton, April 2004)
- “Trend of T_c_max in High-T_c materials? An analysis of t and t' with Wannier functions.”
Department of Physics, BNL (Upton, April 2004)
- “Trend of T_c_max in High-T_c materials? An analysis of t and t' with Wannier functions.”
CMSN workshop (Montreal, March 2004)
- “Trend of T_c_max in High-T_c materials? An analysis of t and t' with Wannier functions.”
APS March Meeting (Montreal, March 2004)
- “Theoretical Perspectives on IXS”
Workshop for NSLS-II: The Future National Synchrotron Light Source (BNL, March 2004)
- “Density Functional Theory, its Extension, and Applications on Solids”
lecture in Department of Physics, SUNY Stony Brook (Stony Brook, October 2003)
- International Workshop on Field Theory Methods in Correlated Nanoscale Systems (BNL, August 2003)
- Strongly Correlated Electrons: NSLS II and the Future (BNL, August 2003)
- “Origin of Magnetic Coupling in Quasi-1D Edge-Sharing Cu-O Chains: Role of the Crystal Potential”
“Dynamical Charge Response of NiO”
“Charge-Transfer Gap of CaB₆: Large Effect of Many-Body Self-Consistency”
APS March Meeting (Austin, March 2003)
- “From weak correlation to strong correlation: *ab initio* many body theory of the next generation”
CMSN workshop (Davis, January 2003)
- “All-Electron, Conserving Investigation of the Band Gap of Si and Ge: Effects of Core States and Many-Body Self-Consistency”
KITP program “Realistic Theories of Correlated Electron Materials” (Santa Barbara, September 2002)
- “Microscopic Analysis of Insulating Magnetism of La₄Ba₂Cu₂O₁₀ and Nd₄Ba₂Cu₂O₁₀”
RERC - Rare Earth Research Conference (Davis, July 2002) (poster)
- Conference on Current Issues in the Optical Response of Solid Materials (Irvine, June 2002)
- “Wannier State Analysis of Insulating Ferromagnetism in La₄Ba₂Cu₂O₁₀”
“All-Electron, Conserving GW calculation of the Quasi-Particle Band Gap in Si and Ge: Effects of the Deep Core States and Many-Body Self-consistency”
ES2002 - Annual Workshop on Recent Developments in Electronic Structure Methods (Berkeley, June 2002) (poster)
- “Microscopic Analysis of Non-Metallic Ferromagnetism in La₄Ba₂Cu₂O₁₀ Based on *Ab Initio* Wannier Functions”
APS March Meeting California session (Davis, March 2002)
- “Microscopic Analysis of Non-Metallic Ferromagnetism in La₄Ba₂Cu₂O₁₀ Based on *Ab Initio* Wannier Functions”
“Dynamical Charge Fluctuations in MgB₂ and the Superconductivity Mechanism”
“Inelastic X-Ray Scattering Investigations of Electron Dynamics in Copper”
“Dynamical Density Response of Metals with Narrow Bands: The Cases of Cr, Ga, and In”
APS March Meeting (Indianapolis, March 2002)
- “*Ab Initio* Investigation of Collective Charge Excitations in MgB₂”
CMSN - Workshop on Excited State Properties and Response Functions for Materials, LBNL (Berkeley, October, 2001)
- ALS / MES / SRRTNet Workshop on Molecular Environmental Science and Theory, Computation and

Synchrotron Experiments, LBNL (Berkeley, October 2001)

- Conference on Strongly Correlated Electron Systems (SCES2001) (Ann Arbor, July 2001)
- “All-Electron, Conserving Investigation of the Band Gap of Si and Ge within the *GW* Approximation”
“Electron-Hole Excitations in Post-Transition Metals Zn and Cd: a Novel Theoretical Perspective”
APS March meeting (Seattle, March 2001)
- “Probing the Electronic Correlations in Condensed Matter with Inelastic Scattering of X-rays”
Division of Material Sciences & Engineering Condensed Matter Physics and Material Chemistry
Program Review, ONRL (Oak Ridge, September 2000) (poster)
- Workshop on Soft X-Ray Science in the Next Millennium: The Future of Photon-In/Photon-Out
Experiments (Pikeville, March 2000)
- “Plasmon Lifetime in K: A Case Study of Correlated Electrons in Solids Amenable to *Ab Initio* Theory”
“Electronic Excitations in Transition Metals of the 3d and 4d Rows with Shallow Core States”
APS March meeting (Atlanta, March 1999)

References

Richard T. Scalettar, *Professor of Physics*

Department of Physics, One Shields Ave., University of California, Davis, CA 95616-8677

Phone: (530) 752-9105 Fax: (530) 752-4717 email: scalettar@physics.ucdavis.edu

Warren E. Pickett, *Professor of Physics*

Department of Physics, One Shields Ave., University of California, Davis, CA 95616-8677

Phone: (530) 752-0926 Fax: (530) 752-4717 email: pickett@physics.ucdavis.edu

Adolfo G. Eguiluz, *Professor of Physics*

Department of Physics, 401 Nielsen Physics Bldg., University of Tennessee, Knoxville, TN 37996-1200

Phone: (865) 974-9642 Fax: (865) 974-7843 email: eguiluz@utk.edu

Bennett C. Larson, *Section Head*

Solid State Division, Oak Ridge National Laboratory, P. O. Box 2008, Oak Ridge, TN 37831-6033

Phone: (865) 574-5506 Fax: (865) 574-4143 email: bcl@ornl.gov

Andrew K. McMahan, *Division Staff Scientist*

H Division, Lawrence Livermore National Laboratory, 7000 East Ave., Livermore, CA 94550-9234

Phone: (925) 422-7198 Fax: (925) 422-2851 email: mcmahan1@llnl.gov

Chi-Chang Kao, *NSLS Associate Chair*

User Science Division, National Synchrotron Light Source, Brookhaven National Laboratory, P.O. Box 5000, Upton, NY 11973-5000

Phone: (631) 344-4494 Fax: (631) 344-3238 email: kao@bnl.gov