

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** **University of Tennessee** Knoxville, TN
1995-2000 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 Award, 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)
- Relevant Experience**
- 2008-present **Brookhaven National Laboratory** Upton, NY
Physicist
- 2003-present **Stony Brook University** Stony Brook, NY
Adjunct Professor
- 2005-2008 **Brookhaven National Laboratory** Upton, NY
Associate Physicist
- 2003-2005 **Brookhaven National Laboratory** Upton, NY
Assistant Physicist
- 2001-2003 **University of California** Davis, CA
Post-graduate Researcher
- 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"
- 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

Skills

All-electron based first-principles many-body theory of condensed matter systems

Ab initio Wannier function analysis of strongly correlated systems

Electronic structure of disordered materials

High-temperature superconductivity

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

Current projects

Disorder-Mediated Properties of Functional Materials

\$960K, Oct. 2010 – Sep. 2013, DOE Office of Science, PI / 6 co-PIs)

Electronic Properties of Transition-Metal-Compound Nanotubes

\$1,230K, Oct. 2011 – Sep. 2014, DOE Office of Science, PI

Previous projects

Electronic properties of transition metal compound nanotubes

\$1230K, 2015 – 2017, DOE, PI

Electronic properties of transition metal compound nanotubes

\$1230K, 2012 – 2014, DOE, PI

Equipment in Support of Predictive Materials Science

\$100K, 20012, DOE, PI

Electronic properties of transition metal compound nanotubes

\$1230K, 2009 – 2011, DOE, PI

Predictive Capability for Strongly Correlated Systems

\$780K, 2007 – 2009, DOE, co-PI / 6 co-PIs

Electronic properties of carbon nanotubes

\$316K, 2006 – 2008, BNL-LDRD, co-PI / 2 co-PIs

Electronic properties of transition metal compound nanotubes

\$1230K, 2006 – 2008, DOE, PI

Predictive Capability for Strongly Correlated Systems

\$780K, 2004 – 2006, DOE, co-PI / 6 co-PIs

Students supervised

Ph.D. students

Dmitri Volja (Physics, Stony Brook University)

Tom Berlijn (Physics, Stony Brook University) – current institute: Oak Ridge National Laboratory

Chia-Hui Lin (Physics, Stony Brook University)

Xugang He (Physics, Stony Brook University)

Co-supervised Ph.D. students

Chi-Cheng Lee (Physics, Tamkang University, Taiwan) – current institute: Academia Sinica, Taiwan

Chen-Lin Yeh (Physics, Tamkang University, Taiwan)

Ryky Nelson (Physics, Louisiana State University)

Chinedu Ekuma (Physics, Louisiana State University)

Postdocs supervised
Weiguo Yin – current institute: Brookhaven National Laboratory
Chi-Cheng Lee – current institute: Academia Sinica, Taiwan
Yucel Yildirim – current institute: Dogus, University, Turkey
Tom Berlijn – current institute: Oak Ridge National Laboratory
Chung-Pin Chou – current institute: Beijing Computational Science Research Center
Limin Wang – current institute: University of Maryland

- Representative Publications**
- “What is the valence of Mn in $\text{Ga}_{1-x}\text{Mn}_x\text{N}$?”
Ryky Nelson, Tom Berlijn, Juana Moreno, Mark Jarrell, and Wei Ku, accepted by Phys. Rev. Lett.
 - “Itinerancy enhanced quantum fluctuation of magnetic moments in iron-based superconductors”
Yu-Ting Tam, Dao-Xin Yao and Wei Ku, Phys. Rev. Lett. **115**, 117001 (2015).
 - “Interpretation of Scanning Tunneling Quasiparticle Interference and Impurity States in Cuprates”
A. Kreisell, *et al.*, Phys. Rev. Lett. **114**, 217002 (2015).
 - “Bulk Signatures of Pressure-Induced Band Inversion and Topological Phase Transitions in $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ ”
Xiaoxiang Xi, *et al.*, Phys. Rev. Lett. **113**, 096401 (2014).
 - “Consequences of broken translational symmetry in $\text{FeSe}_x\text{Te}_{1-x}$ ”
L. Moreschini, *et al.*, Phys. Rev. Lett. **112**, 087602 (2014).
 - “Doping effects of Se vacancies in monolayer FeSe”
Tom Berlijn, Hai-Ping Cheng, P. J. Hirschfeld, and Wei Ku, Phys. Rev. B **89**, 020501(R) (2014).
 - “First-principles method of propagation of tightly bound excitons in LiF: Verifying the exciton band structure with inelastic x-ray scattering”
Chi-Cheng Lee, *et al.*, Phys. Rev. Lett. **111**, 157401 (2013)
 - “Signatures of a pressure-induced topological quantum phase transition in BiTeI”
Xiaoxiang Xi, *et al.*, Phys. Rev. Lett. **111**, 155701 (2013)
 - “Effects of disordered Ru substitution in BaFe_2As_2 : possible realization of superdiffusion in real materials”
Limin Wang, *et al.*, Phys. Rev. Lett. **110**, 037001 (2013)
 - “Temperature-dependent transformation of the magnetic excitation spectrum on approaching superconductivity in $\text{Fe}_{1-x}(\text{Ni}/\text{Cu})_x\text{Te}_{0.5}\text{Se}_{0.5}$ ”
Zhijun Xu, *et al.*, Phys. Rev. Lett. **109**, 227002 (2012)
 - “Effective doping and suppression of Fermi surface reconstruction via Fe vacancy disorder in $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$ ”
Tom Berlijn, P. J. Hirschfeld, and Wei Ku, Phys. Rev. Lett. **109**, 147003 (2012)
 - “Insulating magnetism in vacancy-ordered $\text{K}_{0.8}\text{Fe}_{1.6}\text{Se}_2$ ”
Wei-Guo Yin, Chia-Hui Lin, and Wei Ku, Phys. Rev. B **86**, 081106(R) (2012)
 - “Do transition metal substitutions dope carriers in iron-based superconductors?”
Tom Berlijn, Chia-Hui Lin, William Garber and Wei Ku, Phys. Rev. Lett. **108**, 207003 (2012)
 - “Relevance of the Heisenberg-Kitaev Model for the Honeycomb Lattice Iridates A_2IrO_3 ”
Yogesh Singh, *et al.*, Phys. Rev. Lett. **108**, 127203 (2012)
 - “One-Fe versus Two-Fe Brillouin Zone of Fe-Based Superconductors: Creation of the Electron Pockets via Translational Symmetry Breaking”
Chia-Hui Lin, Tom Berlijn, Limin Wang, Chi-Cheng Lee, Wei-Guo Yin, and Wei Ku, Phys. Rev. Lett. **107**, 257001 (2011)
 - “Kinetics-Driven Superconducting Gap in Underdoped Cuprate Superconductors Within the

Strong-Coupling Limit

Y. Yildirim and Wei Ku, Phys. Rev. X **1**, 011011 (2011)

- “Can disorder alone destroy the e_g hole pockets of $\text{Na}_{0.3}\text{CoO}_2$?”
Tom Berlijn, Dmitri Volja, and Wei Ku, Phys. Rev. Lett. **106**, 077005 (2011)
- “Room temperature magnetism of Cu-doped ZnO films probed by soft X-ray magnetic circular dichroism”
T.S. Heng, *et al.*, Phys. Rev. Lett. **105**, 207201 (2010)
- “A unified picture for magnetic correlations in iron-based high-temperature superconductors”
Wei-Guo Yin, Chi-Cheng Lee, and Wei Ku, Phys. Rev. Lett. **105**, 107004 (2010)
- “Dynamical Linear Response of TDDFT with LDA+U Functional: Strongly hybridized Frenkel excitons in Mott insulators”
Chi-Cheng Lee, Hung-Chung Hsueh, and Wei Ku, Phys. Rev. B **82**, 081106 (R) (2010)
- “Unfolding first-principles band structures”
Wei Ku, Tom Berlijn, and Chi-Cheng Lee, Phys. Rev. Lett. **104**, 216401 (2010)
- “Experimental observation of the crystallization of a paired holon state”
A. Ruydi, W. Ku, *et al.*, Phys. Rev. Lett. **105**, 026402 (2010)
- “Effect of covalent bonding on magnetism and the missing neutron intensity in copper oxide compounds”
Andrew C Walters, *et al.*, Nature Physics **5**, 867 (2010)
- “Charge Ordering in Half-Doped Manganites: Weak Charge Disproportion and Leading Mechanisms”
D. Volja, W.-G. Yin, and Wei Ku, Europhys. Lett. **89** 27008 (2010)
- “Ferro-Orbital Order and Strong Magnetic Anisotropy in the Parent Compounds of Iron-Pnictide Superconductors”
Chi-Cheng Lee, Wei-Guo Yin, and Wei Ku, Phys. Rev. Lett. **103**, 267001 (2009)
- “Tuning Hole Mobility, Concentration, and Repulsion in High-Tc Cuprates via Apical Atoms”
W.-G. Yin and Wei Ku, Phys. Rev. B **79**, 214512 (2009)
- “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, PNAS **105**, 12159 (2008)
- “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, *et al.*, Phys. Rev. Lett. **99**, 026401 (2007)
- “Low-Energy Charge-Density Excitations in MgB₂: 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, *et al.*, 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
- “Surface-state-dominated transport in crystals of the topological crystalline insulator In-doped $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ ”
Ruidan Zhong, *et al.*, Phys. Rev. B **91**, 195321 (2015)
- “First-Principles Studies in Fe-Based Superconductors”
Wei Ku, Tom Berlijn, Limin Wang, and Chi-Cheng Lee, in “Iron-Based Superconductivity” Springer Series in Materials Science 211 (Springer International Publishing Switzerland 2015). ISBN:978-3-319-11253-4. DOI:10.1007/978-3-319-11254-1.
- “Electronic Structure Reconstruction across the Antiferromagnetic Transition in $\text{TaFe}_{1.23}\text{Te}_3$ Spin Ladder”
Min Xu, *et al.*, Chin. Phys. Lett. **32**, 027401 (2015)
- “Coexistence of orbital degeneracy lifting and superconductivity in iron-based superconductors”
H. Miao, *et al.*, Phys. Rev. B **89**, 220503(R) (2014)
- “First-principles Wannier function analysis of the electronic structure of PdTe: weaker magnetism and superconductivity”
Chinedu E Ekuma, Chia-Hui Lin, Juana Moreno, Wei Ku and Mark Jarrell, J. Phys.: Condens. Matter **25**, 405601 (2013)
- “Unusual persistence of superconductivity against high magnetic fields in the strongly-correlated iron-chalcogenide film FeTe_xO_x ”
I.K. Dimitrov, W.D. Si, W. Ku, and S.J. Han, Low Temperature Physics **39**, 680 (2013)
- “Spin-split conduction band in EuB_6 and tuning of half-metallicity with external stimuli”
Jungho Kim, Wei Ku, Chi-Cheng Lee, *et al.*, Phys. Rev. B **87**, 155104 (2013)
- “Magnetic states of the two-leg-ladder alkali metal iron selenides AFe_2Se_3 ”
Qinlong Luo, *et al.*, Phys. Rev. B **87**, 024404 (2013)
- “Thermal evolution of the full three-dimensional magnetic excitations in the multiferroic BiFeO_3 ”
Zhijun Xu, *et al.*, Phys. Rev. B **86**, 174419 (2012)
- “Impact of the two Fe unit cell on the electronic structure measured by ARPES in iron pnictides”

**Other
Publications**

- V. Brouet, *et al*, Phys. Rev. B **86**, 075123 (2012)
- “Itinerant electrons, local moments, and magnetic correlations in the pnictide superconductors $\text{CeFeAsO}_{1-x}\text{F}_x$ and $\text{Sr}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ ”
Paolo Vilmercati, *et al*, Phys. Rev. B **85**, 220503(R) (2012)
 - “Magnetic softness in iron-based superconductors”
Weiguo Yin, Chi-Cheng Lee, and Wei Ku, Supercond. Sci. Technol. **25**, 084007 (2012)
 - “ dd excitations in three-dimensional q -space: A nonresonant inelastic X-ray scattering study on NiO”, N. Hiraoka, M. Suzuki, K. D. Tsuei, H. Ishii, Y. Q. Cai, M. W. Haverkort, C. C. Lee and W. Ku”, Europhys. Lett. **96**, 37007 (2011)
 - “Local-moment magnetism in superconducting $\text{FeTe}_{0.35}\text{Se}_{0.65}$ as seen via inelastic neutron scattering”
Zhijun Xu, Jinsheng Wen, Guangyong Xu, Songxue Chi, Wei Ku, Genda Gu, and J. M. Tranquada, Phys. Rev. B **84**, 052506 (2011)
 - “Nanospheres of a New Intermetallic FeSn(5) Phase: Synthesis, Magnetic Properties and Anode Performance in Li-ion Batteries”
XL Wang, M Feygenson, HY Chen, CH Lin, CH, Wei Ku, JM Bai, MC Aronson, TA Tyson, TA, WQ Han, JACS **133**, 11213 (2011)
 - “Long-range magnetic ordering in Na_2IrO_3 ”
X. Liu, T. Berlijn, W.-G. Yin, W. Ku, A. Tsvelik, Young-June Kim, H. Gretarsson, Yogesh Singh, P. Gegenwart, and J. P. Hill, Phys. Rev. B **83**, 220403(R) (2011)
 - “X-ray diffuse scattering study of local distortions in Fe_{1+x}Te induced by excess Fe”
X. Liu, C.-C. Lee, Z. J. Xu, J. S. Wen, G. Gu, W. Ku, J. M. Tranquada, and J. P. Hill, Phys. Rev. B **83**, 184523 (2011)
 - “Coupling of spin and orbital excitations in the iron-based superconductor $\text{FeSe}_{0.5}\text{Te}_{0.5}$ ”
S.-H. Lee, *et al*, Phys. Rev. B **81**, 220502 (2010)
 - “Nanoscale disorder and local electronic properties of $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$: An integrated study of electron, neutron and x-ray diffraction, x-ray absorption fine structure and first principles calculations”
J.C. Zheng, *et al.*, Phys. Rev. B **81**, 144203 (2010)
 - “Flavored-Twisted Boundary Conditions for the Quantum World: between Big and Small”
Wei-Guo Yin, and Wei Ku, Phys. Rev. B **80**, 180402(R) (2009)
 - “Electronic Properties of Thin Film Periodic Nanostructures”
Travis Sjoström, Daniel C. Mattis, Weiguo Yin, and Wei Ku, J. Comput. Theor. Nanosci. **6**, 403–417 (2009)
 - “GGA+U calculations of correlated spin excitations in LaCoO_3 ”
Karel Knizek, Zdenek Jirak, Jiri Hejmanek, Pavel Novak, and Wei Ku, Phys. Rev. B. **79**, 014430 (2009)
 - “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, Carbon **47** (1), 162 (2009)
 - “A Novel First-Principles Approach to Effective Hamiltonians for high- T_c superconducting cuprates”
Wei-Guo Yin and Wei Ku, JPCS **108**, 012032 (2008) (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)

- “Phonons in superconducting CaC_6 studied via inelastic x-ray scattering”
M. H. Upton, A. C. Walters, C. A. Howard, K. C. Rahnejat, M. Ellerby, J. P. Hill, D. F. McMorro, A. Alatas, Bogdan M. Leu, and Wei Ku, *Phys. Rev. B* **76**, 220501 (2007)
- “Universal quasiparticle decoherence in hole- and electron-doped high- T_c 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 $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ 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)
- “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 TiO_2 ”
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 $\text{La}_4\text{Ba}_4\text{Cu}_2\text{O}_{10}$ and $\text{Nd}_4\text{Ba}_4\text{Cu}_2\text{O}_{10}$ ”
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)
- “ MgB_2 : 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

**Invited
Presentations**

- “Physical effects of disordered impurities on electronic structure of Fe- based superconductors” (ICMAT 2015, Singapore, June, 2015)
- “Phase fluctuation in overdoped cuprates? Superconducting dome due to Mott-ness of the tightly bound preformed pairs” (Superstripes 2015, Ischia, Italy, June, 2015)
- “Physical effects of disordered impurities on electronic structure of Fe- based superconductors” (“Electronic structure approaches & applications to quantum matter”, Las Alamos, May, 2015)
- “Propagation of local excitations in strongly correlated materials” (“Quantum Theory of Materials”, Erlangen, Germany, April, 2015)
- “Connecting real materials to low-energy effective Hamiltonian: applications of symmetry-respecting Wannier functions” (20th Mardi Gras Conference, Baton Rouge, February, 2015)
- “Glide translational symmetry of Fe-based high-temperature superconductors: consequence in the electronic structure and the superconducting pairing structure” (9th international conference of computational physics (ICCP9), Singapore, January, 2015)
- “Spin/Orbital correlation, disordered impurities, and glide translational symmetry of Fe-based superconductors” (minicolloquium on Iron superconductors in the conference “Condensed matter in Paris 2014”, Paris, France, August, 2014)
- “Disordered Impurities and Glide Translational Symmetry in Fe-based Superconductors” (Beijing International Workshop (II) on Iron-Based Superconductors, Beijing, China, July, 2014)
- “The superconducting dome in the cuprates from the strong binding description” (Superstripe 2014, Erice, Italy, June, 2014)
- “Spin/orbital correlation and glide translational symmetry of Fe-based superconductors” (EMN conference on Iron- and Iridium-based superconductivity, Cancun, Mexico, June, 2014)
- “Can high- T_c superconductivity be an entirely different beast under strong correlation?” (University of California at Davis, Davis, May, 2014)
- “Can high- T_c superconductivity be an entirely different beast under strong correlation?” (SLAC, Stanford, May, 2014)
- “Physical effects of disordered impurities on electronic structure of Fe-based superconductors” “Itinerancy enhanced quantum fluctuation of magnetic moments in Fe-based superconductors” (International Conference on Superconductivity and Magnetism 2014, Antalya, Turkey, April, 2014)
- “Can high- T_c superconductivity be an entirely different beast under strong correlation?” (National Taiwan University, Taipei, Taiwan, April, 2014)
- “Propagation of local excitations in strongly correlated materials” “Spin/orbital correlation and glide translational symmetry in Fe-based superconductors” “Physical effects of disordered impurities on electronic structure of Fe-based superconductors” “Can high- T_c superconductivity be an entirely different beast under strong correlation?” (Summer school in National Center of Theoretical Science, Tainan, Taiwan, April, 2014)
- “Physical effects of disordered impurities on electronic structure of Fe-based superconductors” (National Tsinghua University, Shingzhu, Taiwan, April, 2014)
- “Physical effects of disordered impurities on electronic structure of Fe-based superconductors” (5th International Symposium on Electronic and Atomic Structure: The Frontiers of Novel Low-dimensional Materials, Tamsui, Taiwan, April, 2014)
- “Can high- T_c superconductivity be an entirely different beast under strong correlation?”

(22th International symposium on superconductivity, Funabori Japan, November, 2013)

- “Can high- T_c superconductivity be an entirely different beast under strong correlation?”
(University of Tokyo, Tokyo Japan, November, 2013)
- “Can high- T_c superconductivity be an entirely different beast under strong correlation?”
(Riken, Wako Japan, November, 2013)
- “Orbital/spin correlation and doping effects of disordered impurities”
(International workshop on Recent developments in Fe-based high-temperature superconductors, Riverhead, September, 2013)
- “Disordered impurities and strong binding limit of high- T_c ”
(CSRC, Beijing, August, 2013)
- “Recent findings of high- T_c superconductivity”
(BNU, Beijing, August, 2013)
- “Recent findings of high- T_c superconductivity”
(SYSU, Guangzhou, August, 2013)
- “Physical effects of disordered impurities on electronic structure of Fe0superconductors”
(CMP13, Guangzhou, August, 2013)
- “Recent theoretical developments in one-particle spectral function of strongly correlated materials”
(Strong correlations and angle-resolved photoemission spectroscopy, Hamburg, July, 2013)
- “Physical effects of disordered impurities on electronic structure of Fe0superconductors”
(University of Tennessee, Knoxville, July, 2013)
- “What does the rich magnetic structure of Fe-based superconductors tell us? How about effects of the disordered impurities?”
(Oak Ridge National Laboratory, Oak Ridge, July, 2013)
- “Physical effects of disordered impurities on electronic structure of Fe-superconductors”
(WCAM-2013, Suzhou, China, June, 2013)
- “Weak doping dependence of nodal transverse velocity in cuprates”
(Superstripe 2013, Ischia, Italy, May, 2013)
- “Physical effects of disordered impurities on electronic structure of Fe-superconductors”
(2nd International congress on advanced materials, Zhenjiang, China, May, 2013)
- “Propagation of local excitations in strongly correlated materials”
(APS user meeting, Argonne, May, 2013)
- “First-principles Wannier function based methods for disordered materials and applications to studies of oxides and Fe-superconductors.”
(National High Magnetic Field Laboratory, Florida, April, 2013)
- “Kinetic-driven superconducting gap in underdoped cuprate superconductors”
(Renmin University, Shanghai, China, January, 2013)
- “First-principles Wannier function based methods for disordered materials and applications to studies of oxides and Fe-superconductors”
(Fudan University, Shanghai, China, January, 2013)
- “First-principles Wannier function based methods for disordered materials and applications to studies of oxides and Fe-superconductors”
(Computational Science Research Center, Beijing, China, January, 2013)
- “First-principles Wannier function based methods for disordered materials and applications to studies of oxides and Fe-superconductors”
(Tsinghua University, Beijing, China, December, 2012)

- “First-principles Wannier function based methods for disordered materials and applications to studies of oxides and Fe-superconductors”
(Renmin University, Beijing, China, December, 2012)
- “First-principles Wannier function based methods for disordered materials and applications to studies of oxides and Fe-superconductors”
(Institute of Physics, Beijing, China, December, 2012)
- “Kinetic-driven superconducting gap in underdoped cuprate superconductors within the strong-coupling limit”
(Tsinghua University, Beijing, China, November, 2012)
- “Kinetic-driven superconducting gap in underdoped cuprate superconductors within the strong-coupling limit”
(Computational Science Research Center, Beijing, China, November, 2012)
- “Kinetic-driven superconducting gap in underdoped cuprate superconductors within the strong-coupling limit”
(New3SC-9, International Conference on New Theories, Discoveries and Applications of Superconductors and Related Materials, Rome, Italy, September, 2012)
- “Recent progress in treating electronic structure of materials with disordered impurities”
(Theoretical Condensed Matter Physics PI Meeting, Washington, August, 2012)
- “Kinetic-driven superconducting gap in underdoped cuprate superconductors within the strong-coupling limit”
(Superstripes 2012 Quantum Phenomena in Complex Matter, Erice, Italy, July, 2012)
- “First-principles Wannier function based methods for disordered materials and applications to studies of oxides and Fe-superconductors”
(International Symposium and Workshop on Correlated Electrons and Materials Properties of Compounds and Alloys, Porto Heli, Greece, July, 2012)
- “Symmetry-respecting Wannier functions and their applications to strongly correlated condensed matter systems”
(CECAM Workshop on Efficient localised orbitals for large systems, strong correlations and excitations, Cambridge, UK, July, 2012)
- “A journey with Wannier functions starting at UCD: Case studies showing two recent developments”
(Workshop on Novel Materials: Celebrating the 65th Birthday of Warren Pickett, Davis, June, 2012)
- “Recent progress in theoretical/computational methods suitable for studying oxide interfaces”
(Workshop on Recent Progress in Oxide Interfaces, Beijing, China, June, 2012)
- “Computation for physics in real materials”
(Yeshiva University, New York, May, 2012)
- “Computation for physics in real materials”
(Louisiana State University, Baton Rouge, April, 2012)
- “First-principles resolution of two current issues: one-Fe vs. two-Fe picture and effects of transition metal substitution”
(Villa Conference on iron-based superconductors, Orlando, April, 2012)
- “Superconductivity in the strong coupling limit: not your textbook BCS behavior in som many ways”
(Stony Brook University, Stony Brook, April, 2012)
- “Superconductivity in the strong coupling limit: not your textbook BCS behavior in som many

ways”

(University of Florida, Gainesville, March, 2012)

- “First-principles Wannier function based methods for disordered materials and applications to studies of oxides and Fe-superconductors”
APS March meeting (Boston, February, 2012)
- “Unfolding first principles band structure”
“First-principles method for disordered materials”
Workshop on “Computational methods to describe random impurities in solids and disordered alloys”
(University of British Columbia, Vancouver, October 3, 2011)
- “New theoretical findings Fe-based high- T_c superconductors”
E-MRS Symposium: Electronic and magnetic structure of ferropnictide high- T_c superconductors and related compounds
(Warsaw, Poland, September 19, 2011)
- “Recent development of first-principles methods for disordered materials”
(National Center for Theoretical Sciences, Tainan, Taiwan, September 25, 2011)
- “New theoretical findings Fe-based high- T_c superconductors”
International Conference on Novel Superconductivity (Tainan, Taiwan, September 4, 2011)
- “New theoretical findings Fe-based high- T_c superconductors”
OCPA 2011 (Kaohsiung, Taiwan, September 1, 2011)
- “New theoretical findings Fe-based high- T_c superconductors”
2011 Telluride Workshop on Competing Interactions and Colossal Responses in Transition Metal Compounds
(Telluride, Colorado, July 18, 2011)
- “Recent development of first-principles methods”
(Tulane University, New Orleans, May 11, 2011)
- “What do the rich magnetic structures of iron-based superconductors teach us?”
(Louisiana State University, Baton Rouge, May 10, 2011)
- “Recent studies of local excitations in strongly correlated materials”
2011 APS/CNM/EMC Users Meeting (Argonne, Illinois, May 4, 2011)
- “Wave interference of Electrons: Consequences in Broken Symmetry and Anderson Localization in Materials”
Quantum optics and new materials (Beijing, China, January 27, 2011)
- “Ferro-orbital order and magnetic structure in the parent compounds of Fe-based superconductors”
KITP program on “Iron-based Superconductors” (Santa Barbara, California, January 16, 2011)
- “Ferro-orbital order and magnetic structure in the parent compounds of Fe-based superconductors”
(National Center for Theoretical Science, Tainan, Taiwan, October 2010)
- “New first-principles methods: unfolding the band structure and beyond-mean-field approach for disordered system”
(National ChengKung University, Tainan, Taiwan, October 2010)
- “What does the rich magnetic structures of parent compounds tell us about the essential low-energy electronic structure?”
(Nanyang Technological University, Singapore, October 2010)
- “Ferro-orbital order and magnetic structures in the parent compounds of Fe-based

superconductors”

(Tamkang University, Tamsui, Taiwan, September 2010)

- “Strong coupling picture of superconductivity in underdoped cuprates”
(Tamkang University, Tamsui, Taiwan, September 2010)
- “Ferro-orbital order and magnetic structure in the parent compounds of Fe-based superconductors”
(National ChingHua University, Sinchu, Taiwan, September 2010)
- “Ferro-orbital order and magnetic structure in the parent compounds of Fe-based superconductors”
(National Taiwan University, Sinchu, Taiwan, September 2010)
- “What does the Ferro-orbital order and magnetic structures in the parent compounds of Fe-based superconductors”
(Academia Sinica, Taipei, Taiwan, September 2010)
- “Advanced first-principles calculations and many-body effects in correlated materials”
QS²C Theory Forum (RIKEN Wako, Saitama, Japan, September 2010)
- “What does the rich magnetic structures of parent compounds tell us about the essential low-energy electronic structure?”, international workshop on “Electronic Structure of Fe-based Superconductors” (MPI Stuttgart, Germany, May 2010)
- “Simplifying local excitations in correlated charge transfer insulators”
LASSP, Cornell University (Ithaca, New York, October 2009)
- “A new first-principles method for electronic structure of disordered materials”
“Ferro-orbital order and strong magnetic anisotropy in the parent compounds of Fe-pnictides superconductors”
University of Florida (Gainesville, Florida, October 2009)
- “A new first-principles method for electronic structure of disordered materials”
workshop on “Characterization of Advanced Materials Under Extreme Environments for the Next Generation Energy Systems” (Brookhaven National Lab, New York, September 2009)
- “Ferro-orbital order and strong magnetic anisotropy in the parent compounds of Fe-pnictides superconductors”
International Workshop on “Frontiers in Density Functional Theory” (Montauk, New York, September 2009)
- “Simplifying local excitations in correlated charge transfer insulators”
GRC “X-Ray Science” (Waterville, Maine, August 2009)
- “Local excitations in strongly correlated charge transfer insulators”
“Second International Symposium and Workshop on Correlated Electrons in Matter” (Gatlinburg, Tennessee, April 2009)
- “Ferro-orbital order and strong magnetic anisotropy in the parent compounds of Fe-pnictides superconductors”
Max-Planck Institute (Stuttgart, Germany, March 2009)
- “Local excitations in strongly correlated charge transfer insulators”
DPG 2009 “Ab-initio approaches to excitations in condensed matter” (Dresden, Germany, March 2009)
- “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 X-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 Hole 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 Hole Mobility, Concentration, and Repulsion in High- T_c Cuprates via Apical Atoms”
CMSN workshop (Denver, 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-Tc 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)
- Presentations/
Conferences**
- “Phase fluctuation in overdoped cuprates? Superconducting dome due to Mott-ness of the tightly bound preformed pairs”
“Generic Symmetry Breaking Instability of Topological Insulators due to a Novel van Hove Singularity”
“Itinerancy enhanced quantum fluctuation of magnetic moments in iron-based superconductors”
“Searching for ideal bulk insulating Pb-system topological crystalline insulator materials”
APS March Meeting (San Antonio, March 2015)
 - “Glide translational symmetry of Fe-based high-temperature superconductors: consequence in the electronic structure and the superconducting pairing structure”
(KITP_2014: Magnetism, Bad Metals and Superconductivity: Iron Pnictides and Beyond, Santa Barbara, September, 2014)
 - “Phase fluctuation in overdoped cuprates? Superconducting dome due to Mott-ness of the tightly bound preformed pairs illustrated via Gutzwiller approximation”
(CECAM workshop on Gutzwiller wavefunctions and related methods, Valence, France, June, 2014)
 - “Physical effects of disordered impurities on electronic structure of Fe-based superconductors”
“Itinerancy enhanced quantum fluctuation of magnetic moments in Fe-based superconductors”
(International Conference on Superconductivity and Magnetism 2014, Antalya, Turkey, April, 2014)
 - “Observation of acoustic-phonon-like mode driven by magnetic imbalance between neighboring Fe atoms in $\text{Fe}_{1+y}\text{Te}_{y<0.12}$ ”
“Probing the pressure-induced topological phase transition in BiTeI”
“Weak phase stiffness and nature of the quantum critical point in underdoped cuprates”
“Do Se vacancies electron dope monolayer FeSe?”
“Coexistence of orbital degeneracy lifting and superconductivity in iron-based superconductors”
“Orbital-Parity Selective Superconducting Pairing Structures of Fe-based Superconductors under Glide Symmetry”
“Detecting topological phase transitions of insulators in the complex crystal momentum space”
“Itinerancy enhanced quantum fluctuation of magnetic moments in iron-based superconductors”
“What is the valence of Mn in GaMnN?”
APS March Meeting (Denver, March 2014)
 - “Weak doping dependence of nodal transverse velocity in underdoped cuprates: explanation and significant implications”
“Effective doping and suppression of Fermi surface reconstruction via Fe vacancy disorder in $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$ ”

“Glide symmetry of iron-based superconductors: Electronic structure and superconductivity”
 “Block versus Stripy Antiferromagnetism in the Fe-Based Spin-Ladder Materials (Ba,K)Fe₂Se₃”
 “Create Dirac Cones in Your Favorite Materials”
 “Inelastic neutron scattering studies on the incommensurate-to-commensurate transformation of low energy magnetic excitations in Fe_{-1+d-y}(Ni/Cu)_yTe_{1-x}Se_x”
 “Magnetic States of the Two-Leg Ladder Iron Selenides”
 “Effects of disordered Ru substitution in BaFe₂As₂: possible superdiffusion mechanism in real materials”
 “Does the physics of (Ga,Mn)N differ from (GaMn)As qualitatively or quantitatively? Is valance of Mn impurity 2+ or 3+?”
 APS March Meeting (Baltimore, March 2013)

- “Wavelets for everything”
 (LSU CCT “Crazy Interdisciplinary Ideas Seminar Series”, August, 2012)
- “Spin/orbital correlation of Fe-based superconductors and first-principles resolution of two current issues: one-Fe vs. two-Fe picture and effects of transition metal substitution”
 (1st Annual World Congress of Advanced Materials, Beijing, China, June, 2012)
- “Dynamical Cluster Approximation: Cluster Extension of CPA for Disordered System”
 “One-Fe versus Two-Fe Brillouin Zone of Fe-Based Superconductors: Creation of the Electron Pockets via Translational Symmetry Breaking”
 “First-Principle Calculation of The Effective Hamiltonian for (Ga,Mn)As and (Ga,Mn)N”
 “Effects of disordered isovalent substitution in Fe-based superconductor”
 “Anisotropic field-induced melting of orbital ordering phase in Pr_{0.6}Ca_{0.4}MnO₃”
 “Novel Magnetism in K_{0.8}Fe_{1.6}Se₂ Explained in the Unified Picture”
 “Do Transition Metal Substitutions Dope Carriers in Iron Based Superconductors?”
 “Unusual Persistence of Superconductivity Against High Magnetic Fields in the Strongly-Correlated Iron-Chalcogenide Film FeTe:O_x”
 “Kinetics-Driven Superconducting Gap in Underdoped Cuprate Superconductors Within the Strong-Coupling Limit”
 APS March Meeting (Boston, February 2012)
- “Observation of room-temperature ferromagnetism in Cu:ZnO films part II; a theoretical study”
 “Observation of room-temperature ferromagnetism in Cu:ZnO films part I; soft X-ray Magnetic Circular Dichroism”
 “A TDLDA+U approach on strongly hybridized Frenkel excitons in Mott insulators and implications to TDDFT and GW+BSE”
 “Evidence for local moment magnetism in superconducting FeTe_{0.35}Se_{0.65}”
 “Unified Picture for Magnetic Correlations in Iron-Based Superconductors”
 “Lifshitz transition in *c*/16 Li at high pressures: Unfolding first-principles Fermi surfaces”
 “Unfolding first-principles band structures”
 “Two-dimensional dynamical reconstruction of the valence exciton in LiF”
 APS March Meeting (Dallas, March 2011)
- “What does the rich magnetic structures of Fe-based high-T_c materials tell us about the essential low-energy electronic structure?”, Superstripes2010 (Erice, Italy, July 2010)
- “Ferro-Orbital Order and Anisotropic Magnetic Structure in Parent Compounds of Iron Pnictides”
 “Functional minimization scheme for first-principles electronic structure calculations with bi-orthogonal interpolating wavelets”
 “Strong coupling picture of superconductivity in underdoped cuprates II: quasi-particle gap and its symmetry”

“Strong coupling picture of superconductivity in underdoped cuprates I: weak phase stiffness and mass divergence of d-wave superfluid”

“Effect of covalent bonding on magnetism and the missing neutron intensity in cuprates”

APS March Meeting (Portland, March 2010)

- “Simplifying local excitations in correlated charge transfer insulators”
KITP “From Basic Concepts to Real Materials” (Santa Barbara, California, November 2009)
- “Structural, spin, and orbital phase transitions in LaOFeAs: I. Total energy calculations”
“Structural, spin, and orbital phase transitions in LaOFeAs: II. Wannier function analysis”
“Local excitations in charge-transfer insulators: a super atom approach via Wannier functions”
“Does disorder destroy e_g ’ pockets in $\text{Na}_{0.3}\text{CoO}_2$? A new ab initio method for disorder”
“Strong coupling limit of superconductivity in anti-ferromagnetic phase: Extended hardcore boson picture of d-wave order and phase fluctuation”
“Functional minimization scheme for first-principles electronic structure calculations with bi-orthogonal interpolating wavelets”
APS March Meeting (Pittsburgh, March 2009)
- “Strong Coupling Limit of Superconductivity: an extended hardcore boson picture for cuprates”
BNL (Upton, August 2008)
- “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- T_c Cuprates via Apical Atoms”
“Phonon Softening and Displacement Pattern in Commensurate Charge Density Wave in 2H-TaSe_2 ”
“Phase Fluctuations in high- T_c Superconductors”
“Strong hybridization of Frenkel excitons in Mott insulators: a novel Wannier function perspective”
“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 MnF_3 : 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 MnF_3 : 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

Ole K. Andersen, *Professor*

Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart, Germany

Phone: +49 711 689 16 30 email: oka@fkf.mpg.de

Elbio R. A. Dagotto, *Distinguished Professor*

Department of Physics, University of Tennessee, 401 Nielsen Physics Building, 1408 Circle Drive,
Knoxville, TN 37996-1200

Phone: (865) 974-2122 email: edagotto@utk.edu

Mark Jarrell, *Professor*

Department of Physics & Astronomy, Louisiana State University, 285 Nicholson Hall, Tower Dr.,
Baton Rouge, LA 70803-4001

Phone: (225) 578-7528 email: jarrellphysics@gmail.com

Peter Hirschfeld, *Professor*

Department of Physics, P.O. Box 118440, Gainesville, FL 32611-8440

Phone: (352) 392-8749 email: pjh@phys.ufl.edu

Philip Phillips, *Professor*

Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street Urbana,
IL 61801-3080

Phone: (217) 244-2003 email: dimer@illinois.edu

Igor Mazin, *Research Scientist*

Center for Computational Material Science, NRL, code 6390, 4555 Overlook Ave SW, Washington,
DC 20375

Phone: (202) 767-6990 email: mazin@nrl.navy.mil

Richard T. Scalettar, *Professor*

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

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

Peter Abbamonte, *Associate Professor*

Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street Urbana,
IL 61801-3080

Phone: (217) 244-4861 email: abbamont@illinois.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 email: bcl@ornl.gov

Chi-Chang Kao, *Director*

Stanford Synchrotron Radiation Light Source SLAC National Accelerator Laboratory, 2575 Sand Hill
Road Menlo Park, CA 94025

Phone: (650) 926-3699 email: ckao@slac.stanford.edu