Report: June 19, 2012

24th Annual Workshop on Recent Developments in Electronic Structure Theory

I. Overview

ES12: The *24th Annual Workshop on Recent Developments in Electronic Structure Theory* was held June 5-8, 2012 at Wake Forest University in Winston-Salem, NC 27109. Starting in 2010, the local organizing committee, consisting of Timo Thonhauser, Natalie Holzwarth, and Akbar Salam worked together to organize the conference and make the local arrangements. They also worked with the international steering committee to choose a list of topics representing recent major developments in the field and invited speakers. The program consisted of 24 oral presentations, 70 posters, and 2 panel discussions. The attendance of the Workshop was comparable to or larger than previous workshops and participation was impressively diverse. Participants came from all over the world and included undergraduate students, graduate students, postdoctoral researchers, and senior scientists. The general assessment of the Workshop was extremely positive in terms of the high level of scientific presentations and discussions, and in terms of the schedule, accommodations, and affordability of the meeting. Several participants, including former organizers, offered very complimentary remarks at the end of the conference. Our ES12 workshop was featured on the front page of Wake Forest University's webpage, and was picked up by *The Business Journal* and the phys.org webpages.

In the following report, Section II lists the organizers of the Workshop, Section III describes the program, Section IV describes the statistics of the participants, and Section V describes some details of the venue of the Workshop. Information about the funding sources is given in Section VI. The program schedule for the workshop, a list of poster presentations, and a list of participants are given in Section VII. More information is available on the ES12 webpage at http://es12.wfu.edu. We intend to keep this webpage available for reference. The abstracts and PDF files from ES12 will also be archived at the Materials Computation Center Website of the University of Illinois.

II. Workshop Organizers

Local Organizing Committee:

- Timo Thonhauser, Department of Physics, Wake Forest University
- Natalie Holzwarth, Department of Physics, Wake Forest University
- Akbar Salam, Department of Chemistry, Wake Forest University

In addition, invaluable assistance was given by Debra Alty and her staff in the Provost's Office, and the Wake Forest University Conference Services Department. We are also grateful to several Wake Forest University staff and students including Gloria Stickney, Eric Chapman, Piero Canepa, Brian Kolb, Nicholas Lepley, Graham Lopez, David Montgomery, David Beck, Daniel Johnson, and Sina Zolghadr.

The Electronic Structure Workshop Series is directed by the following steering committee:

- Stefano Baroni, SISSA, Trieste, Italy
- Jerry Bernholc, North Carolina State University
- Roberto Car, Princeton University
- Jim Chelikowsky, University of Texas
- David M. Ceperley, University of Illinois
- Mei-Yin Chou, Georgia Institute of Technology
- Jim Gubernatis, Los Alamos National Lab
- Duane Johnson, Iowa State University
- Steve G. Louie, University of California, Berkeley
- Richard M. Martin, University of Illinois
- Warren Pickett, University of California, Davis
- Andrew Rappe, University of Pennsylvania
- Cyrus J. Umrigar, Cornell University
- David Vanderbilt, Rutgers University

The steering committee met with the local organizing committee in February 2012 at the venue of the American Physical Society meeting to discuss the topics and potential speakers for the ES12 Workshop.

III. Program

There was a Welcome Reception for all participants on the evening of Tuesday, June 5th at Polo Residence Hall. The program of Oral Presentations started at 8:15 am on Wednesday, June 6th in Pugh Auditorium. Posters were available in Benson 401 throughout the Workshop. Poster presenters of even-numbered posters were available for Poster Session A on Wednesday afternoon, while poster presenters of odd-numbered posters were available for Poster Session B the following afternoon. The conference Banquet took place on Wednesday evening. On Thursday evening, a Discussion Forum on topics of interest to the electronic structure community was held in the Byrum Welcome Center, followed by a dessert reception. The full schedule for the meeting is given in Section VI.

The practice of including panel discussions as part of the Workshop program was initiated by Andrew Rappe at ES11 held at the University of Pennsylvania. We decided to continue this practice for ES12. The panel discussions on Thursday evening were attended by roughly 60

participants in addition to the 12 panel members. The experience of the panel discussions from both ES11 and ES12 encourage continuing dialog which will hopefully eventually lead to practices which will benefit the Materials Modeling community.

The first panel on "Strategies for continued support of public domain code collaborations such as abinit, quantum espresso, etc." had panelists representing the abinit, quantum espresso, conquest, and socorro collaborations in addition to two panelists involved with several code projects in a variety of capacities. While the discussion did not result in a consensus, several key points were made.

- Most agreed that it is important to encourage students to get involved with code development and testing. If a student has developed a new feature in one of the packages, it is often good to encourage the student to perform the extra step of adding the feature to the package distribution so that others can benefit from the work.
- Some details of how to ensure code integrity were discussed. This depends on the organization and the development of "rules" within each collaboration.
- Several of the panelists from Europe discussed European based initiatives for collaborative computation efforts. It appears that similar initiatives in the United States have not been so focused or effective. In the United States, there does not seem to be an organizational or funding mechanism for long-term code collaborations.
- There was a brief discussion of dft++ originally developed at Cornell University as a high level language for facilitating the implementation of computational ideas. Apparently, new versions of this high level language are being revisited at Cornell and there appears to be considerable interest both among the developers and potential users.
- One suggestion was that it might be useful to examine the existing code collaborations to develop a sense of "best practices" for successful collaborations. This may or may not include closer collaboration between theoretical physicists and chemists with mathematicians and computer scientists. It may or may not include attempts at standardization with a view to sharing information between codes or, at the other extreme, developing contributions in the form of libraries that could be used in other codes.
- An issue which had broad support was that there should be incentives or rewards for efforts invested in good code development. Often code developers have shorter publications lists and apparent productivity than those who primarily use codes developed by others.

The second panel on "Advocacy for a new topical group for Electronic Structure Computation at the American Physical Society" had some overlap with the first panel, but generally was a broader discussion.

- The panelists and audience seem to be evenly divided on whether it would be better to develop a US version of the European Psi-k Organization which now is an non-governmental non-profit organization, or to pursue a topical group designation through APS. The latter has the advantage of an existing organizational structure while the former has more flexibility in general and is more naturally interdisciplinary.
- Some activities of a materials-modeling advocacy group might be

    - Find ways to encourage good code development such as institute prizes or other honors for exemplary achievement
    - Develop training courses on simulation methods, not always tied to a particular software package
    - Provide databases of inputs and outputs for some subset of the calculations; more generally find ways to promote collaborative work
    - Providing general advocacy for materials simulations. While it seems difficult to imagine that we can (or should) agree on a single vision or "road map" for the field, it may be that regular consultation among our group could be beneficial. For example there is the potential for positive impact on policy and/or funding decisions, etc.
- Toward the end of the discussion it was noted that should this forum continue in succeeding years, additional direct student input might be desirable.
- While it was not mentioned in the panel discussions, it might be productive to continue the dialog we have started in an online forum of some sort.

IV. Workshop Data and Statistics

The approximate number of registered participants of the Workshop was 136. In addition, there were several local non-registered attendees. Of the 136 registrants, 5 were undergraduate students, 54 were graduate students, 25 were postdoctoral researchers, and the rest were faculty or industrial or government researchers. Of the 136 registrants, one traveled from Taiwan, 2 traveled from Colombia, 1 traveled from Brazil, 11 traveled from Europe, 1 traveled from Canada, and the rest traveled from various parts of the United States. Of the 24 speakers, 2 were graduate students, 5 were postdoctoral research associates and 17 were faculty or government researchers, with 4 of the speakers female. In other demographical designations—of the 24 speakers, 7 were from Europe while 17 were from US or Canada.

V. Workshop Venue and Practices

The oral presentations for the Workshop were given in Pugh Auditorium in the Benson University Center, which provided comfortable seating for the participants. The posters were mounted on easels in Room 401 of the Benson University Center, which had a large enough space for all 70 easels plus discussion space. The panel discussions were held in a new auditorium at the Porter Byrum Welcome Center.

The oral presentations were 30 minutes with 5 minutes for discussion arranged in 8 topical groups—Challenging Materials; Simulations of Phase Transitions; Large Scale Simulations and Materials Design; Developments in Density Functional Theory; Beyond DFT; Quantum Monte Carlo; Partitioning, Embedding, and Complex Systems; and Topological Insulators. The posters were available throughout the meeting; the program allowed for two 1.5 hour periods for poster discussions. Four posters presented by graduate students and 1 poster presented by a postdoctoral researcher were awarded a prize. Each prize winner received a copy of Richard Martin's monograph *Electronic Structure: Basic Theory and Practical Methods.*

Because of the generous support from funders, the registration costs for the conference could be kept very low. The basic registration cost (waived for invited speakers) was $251 including room and board (3 nights in Polo Residence Hall). Late registration (after May 15th) was increased by $50. The fee collection was managed by the Professional Development Center at Wake Forest University. The Workshop fee was one of the lowest in the past several years, which was partly responsible for the success in terms of workshop attendance.

The workshop provided meals on campus at The Fresh Food Company. In addition, there was a reception on Tuesday evening at the Polo residence hall, a banquet on Wednesday evening at the Magnolia Room in Reynolda Hall, and a dessert reception on Thursday evening at the Porter Byrum Welcome Center. Beverages and snacks were provided between oral presentations and during the poster sessions. The Workshop provided airport shuttle service between campus and the Greensboro International Airport (GSO) on Tuesday and Friday afternoons. The Workshop participants received a carrying bag containing the printed program and other information.

VI. Funding sources

- Wake Forest University, Office of the Provost
- Wake Forest University, Departments of Physics and Chemistry
- Materials Computation Center, University of Illinois, Supported by NSF Award DMR 11-07472
- Army Research Office
- The Department of Energy
- Robert BOSCH LLC Research and Technology Center North America (supported the conference banquet)

The ARO, DOE, and NSF funds were used to support the conference fees and travel reimbursements for the invited speakers, printing costs for conference information, airport shuttle costs, and poster prizes.

VII. Program Schedule, Poster Presentations, and List of Participants

Program Schedule

Wednesday, June 6, 2012
7:00 am - 8:00 am, Breakfast, Fresh Food Company
Coffee/Tea/Refreshments available in lobby of Pugh Auditorium starting at 7:30 am

8:15 am	Timo Thonhauser *Wake Forest University*	Opening Remarks
8:20 am	Mark Welker *Interim Provost and William L. Poteat Professor of Chemistry, Wake Forest University*	Welcome

Plenary Session I: Challenging Materials
Session chair: Mei-Yin Chou, *Academia Sinica*

8:30 am	Oana Jurchescu *Wake Forest University*	An Experimental Perspective: Tailoring Crystalline Order in Organic Thin-Film Transistors by Exploring Interactions at Interfaces
9:05 am	Noa Marom *University of Texas at Austin*	Electronic Structure of Dye-Sensitized TiO2 Clusters from *G0W0*
9:40 am	Pieremanuele Canepa *Wake Forest University*	Sequestration and Diffusion of Small Non-Polar Molecules in MOF Materials

10:15 am - 10:45 am, Coffee break

Plenary Session II: Simulations of Phase Transitions
Session chair: David Ceperley, *University of Illinois, Urbana-Champaign*

10:45 am	Marc Torrent *CEA, France*	Dense Hydrogen by First-Principles Path-Integral Molecular Dynamics: Structure of Phase II, Melting Curve, and Beyond
11:20 am	Jeff McMahon *University of Illinois*	On the Molecular Dissociation of Dense Hydrogen and the Solid/Liquid Transition in the Atomic Phase via Free-energy Calculations
11:55 am	Daniel Sheppard *Los Alamos National Laboratory*	A Generalized Solid-State Nudged Elastic Band Method

12:30 pm - 2:00 pm, Lunch, Fresh Food Company

Poster Session A: 2:00 pm - 3:30 pm in Room 401 of Benson University Center
Coffee/Tea/Refreshments available in 401 Benson starting at 2:00 pm

Plenary Session III: Large Scale Simulations and Materials Design
Session chair: Alan F. Wright, *Sandia National Laboratories*

3:45 pm	David Bowler *University College London, England*	Recent Developments in the Linear Scaling DFT code CONQUEST: Constrained DFT, TDDFT, and Basis Sets
4:20 pm	Joseph Bennett *Rutgers University*	The Discovery and Design of Multifunctional Materials: Integration of Database Searching and First Principles Calculations
4:55 pm	Cai-Zhuang Wang *Iowa State University*	Adaptive Genetic Algorithm Method for Crystal Structure Prediction and Materials Discovery

Cocktail Reception & Musical Entertainment
6:30 pm - 7:30 pm, Green Room, Reynolda Hall

Conference Banquet
7:30 pm - 9:30 pm, Magnolia Room, Reynolda Hall
The conference banquet is kindly sponsored by the
Robert BOSCH LLC Research and Technology Center North America

Thursday, June 7, 2012

7:00 am - 8:00 am, Breakfast, Fresh Food Company
Coffee/Tea/Refreshments available in lobby of Pugh Auditorium starting at 7:30 am

Plenary Session IV: Developments in Density Functional Theory
Session chair: Normand Modine, *Sandia National Laboratory*

8:30 am	Nicola Marzari *EPFL, Switzerland*	Density-Functional Theory: Time to Move On?
9:05 am	Andreas Görling *University of Erlangen-Nuremberg, Germany*	The Adiabatic-Connection Dissipation-Fluctuation Theorem as Route to a New Generation of Density-Functional Methods
9:40 am	Rodney J. Bartlett *University of Florida*	Is There a Consistent Density Functional Theory?

10:15 am - 10:45 am, Coffee break

Plenary Session V: Beyond DFT -- GW, Time-dependence, EM fields
Session chair: Jerry Bernholc, *North Carolina State University*

10:45 am	Josef Zwanziger *Dalhousie University, Canada*	Homogeneous Electric and Magnetic Fields in Periodic Systems
11:20 am	Stefano Baroni *SISSA, Italy*	*Ab Initio* Colors
11:55 am	Sohrab Ismail-Beigi *Yale University*	Progress and Challenges with Luttinger-Ward Approaches for Going Beyond DFT

12:30 pm - 2:00 pm, Lunch, Fresh Food Company

Poster Session B: 2:00 pm - 3:30 pm in Room 401 of Benson University Center
Coffee/Tea/Refreshments available in 401 Benson starting at 2:00 pm

Plenary Session VI: Quantum Monte Carlo
Session chair: Cyrus Umrigar, *Cornell University*

3:45 pm	Claudia Filippi *University of Twente, The Netherlands*	Size-Extensive Wave Functions for Quantum Monte Carlo: A Linear Scaling Generalized Valence Bond Approach

4:20 pm	Bryan Clark *Princeton University*	Approaching Strongly Correlated Systems using Partial Node FCIQMC
4:55 pm	Shiwei Zhang *College of William and Mary*	Auxiliary-Field Quantum Monte Carlo Calculations of Excited States and Strongly Correlated Systems

6:00 - 7:30 pm, Dinner, Fresh Food Company

Community Panel Discussions & Dessert
7:30 pm - 10:00 pm, Byrum Auditorium

- Strategies for continued support of public domain code collaborations such as *abinit, quantum espresso,* etc. *Panelists: Stefano Baroni, David Bowler, Jeongnim Kim, Nicola Marzari, Marc Torrent, David Vanderbilt, Alan Wright, and Josef Zwanziger*
- Advocacy for a new topical group for Electronic Structure Computation at the American Physical Society. *Panelists: Jerry Bernholc, David Ceperley, Mei-Yin Chou, Nicola Marzari, and Andrew Rappe*

Friday, June 8, 2012

7:00 am - 8:00 am, Breakfast, Fresh Food Company
Coffee/Tea/Refreshments available in lobby of Pugh Auditorium starting at 7:30 am

Plenary Session VII: Partitioning, Embedding, and Complex Systems
Session chair: Jeongnim Kim, *Oak Ridge National Laboratory*

8:30 am	Lai Jiang *University of Pennsylvania*	Electrons on a Leash: Topology-based Charge Partitioning and Rigorous Definition of Oxidation States in Solids
9:05 am	Garnet Chan *Princeton University*	Density Matrix Entanglement Embedding for Strongly Correlated Electronic Structure
9:40 am	Renata Wentzcovitch *University of Minnesota*	Spin Crossover Systems in the Deep Mantle

10:15 - 10:45 am, Coffee break

Plenary Session VIII: Topological Insulators
Session chair: David Vanderbilt, *Rutgers University*

10:45 am	Raffaele Resta *University of Trieste, Italy*	Topological Order in Electronic Wavefunctions
11:20 am	Andrew Rappe *University of Pennsylvania*	Dirac Semimetal in Three Dimensions
11:55 am	Alexey Soluyanov *Rutgers University*	First-Principles Calculation of Topological Invariants

12:30 pm	Natalie Holzwarth *Wake Forest University*	Closing Remarks

12:45 pm - 2:00 pm, Lunch, Fresh Food Company (lunch boxes available)

Poster Presentations

#36 M. Aminpour *University of Central Florida*	Physisorption of Three Amine Terminated Molecules (TMBDA, BDA, TFBDA) on the Au(111) Surface: The role of van der Waals Interactions	poster
#37 T. Berlijn *Brookhaven National Laboratory*	Effects of Disordered Substitutions and Vacancies In Fe Based Superconductors from First Principles	
#38 T. Birol *Cornell University*	Structural and Electronic Trends in Rutile Compounds	
#39 A. Cancio *Ball State University*	Laplacian-Based Models for the Exchange Energy	poster
#40 T. Cheiwchanchamnangij *Case Western Reserve University*	Quasiparticle Band Structure Calculations of Monolayer, Bilayer, and Bulk MoS2	poster
#41 Z. Chen *University of Massachusetts at Amherst*	Spectral Propagation Schemes for TDDFT Calculations with Applications to Molecules and CNT's	poster
#42 R. Longo-Pazos *The University of Texas at Dallas*	Intrinsic Voltage Limit and Crystal Field Splitting in Silicate Cathode Materials for Li-Ion Batteries	poster
#43 H. Das *Cornell University*	First Principles Investigation of Structural and Electronic Properties of Hexagonal Rare-Earth Ferrites, RFeO3 (R=Lu-Tm)	poster
#44 M. Fellinger *The Ohio State University*	Ab Inito-Based Interatomic Potentials for Body-Centered Cubic Refractory Metals	
#45 K. Garrity *Rutgers University*	Modeling Piezoelectricity in Improper Ferroelectrics	
#46 B. Gavin *University of Massachusetts at Amherst*	A Nonlinear Eigensolver-Based Alternative to Traditional SCF Methods	poster
#47 S. Ghosh *Cornell University*	Above Room Temperature Ferroelectricity and Weak Ferromagnetism in LaFeO3/LnFeO3 Hybrid Improper Ferroelectrics	poster

#48 Z. Goldsmith *University of Pennsylvania*	Constructing an Improved Ce Pseudopotential in OPIUM Code	poster
#49 R. Gonzalez-Hernandez *Universidad del Norte, Colombia*	Interface Formation of Scandium Nitride on GaN(0001) Surface: A First-Principle Study	poster
#50 Y. Guo *University of Cambridge, UK*	Metal-Insulator Transition of V2O3 from Screened Hybrid Functional	poster
#51 N. Holzwarth *Wake Forest University*	First Principles Computer Simulations of Li10GeP2S12 and Related Lithium Superionic Conductors	poster
#52 J. Hong *Rutgers University*	Spin-Phonon Coupling Effects in Transition-Metal Perovskites: A DFT+U and Hybrid-Functional Study	poster
#53 S. Hong *University of Central Florida*	Rationale for the High Reactivity of the Interfacial Sites in Methanol Oxidation on Au/TiO2	
#54 L. Huang *Case Western Reserve University*	CsSnX3 Band Structure Calculations by the QSGW method	poster
#55 S. Huang *Washington University*	Lattice Vibrational Modes in Si/Ge Core-shell Nanowires	poster
#56 J. Jiang *Yale University*	Nanoscale Photovoltaics: Aminoethanethiol Coated CdSe Quantum Dots	poster
#57 A. Kabir *University of Central Florida*	Magnetic Properties of Transition Metal Nanoparticles: A DFT-Inhomogeneous-DMFT Analysis	poster
#58 A. Kakekhani *Yale University*	Ferroelectric Surface Chemistry: First Principle Study of Nox Decomposition	
#59 A. Kara *University of South Florida*	Adsorption Characteristics of Acenes on Cu(110) and Ag(110)	
#60 A. Kaur *University of California Davis*	Core Polarization Effects from Dielectric Eigenpotentials	
#61 J. Kestyn *University of Massachusetts at Amherst*	Real-Space All-Electron Band Structure Calculations	poster
#62 S. Kim *University of Pennsylvania*	Strong Dependence of Oxide Work Functions on Surface Structures	
#63 B. Kolb *Wake Forest University*	Teaching Computers to be Physicists: Machine Learning with Network Functions	poster

#64 B. Kozinsky *Robert Bosch LLC*	Ab Initio Spectroscopy and Screening of Materials for Li/Air Batteries	
#65 J. Lee *Cornell University*	Two-Level States In Substitutional Mixed Crystal: Ab Initio Predictions for Glass Transitions	
#66 N. Lepley *Wake Forest University*	Computer Modeling of Crystalline Electrolytes - Lithium Thiophosphates and Phosphates	poster
#67 K. Letchworth-Weaver *Cornell University*	Surface Studies with Combined Free Energy Functionals of Electronic and Liquid Densities (grad student prize)	poster
#68 Y. Liang *Washington University*	Enhanced Many-Electron Effects in Gated Bilayer Graphene	poster
#69 Q. Li *Wake Forest University*	Transport of Hot Electrons in Scintillators: NaI and SrI2	
#70 Q. Li *Wake Forest University*	First Principles Calculations of Iodine Vacancy Centers in SrI2	poster
#71 Y. Liu *Rice University*	Edges of Low-dimensional Materials: Structures, Energies, and Applications	
#72 M. Lopez *Wake Forest University*	Ab Initio Calculation of Indirect Spin-Spin Coupling Constants	poster
#73 W. Lopez-Perez *Universidad Del Note, Colombia*	Ab Initio Study of the Structural and Electronic Properties of Zr Adsorption on AlN (0001) Surface	poster
#74 D. Lu *Brookhaven National Laboratory*	Beyond RPA Correlation Energies: Evaluation of Model Exchange-Correlation Kernels	
#75 C. Martins *CEA, France*	Spin-Orbit Coupling within Dynamical Mean-Field Theory: Coulomb Correlations in 4d and 5d Transition Metal Oxides	poster
#76 M. Mendez Polanco *University of Pennsylvania*	Adsorption of Alanine on Ferroelectric Surfaces (grad student prize)	
#77 N. Modine *Sandia National Laboratories*	Reconstruction and Disorder at Compound Semiconductor Surfaces	
#78 J. Moussa *Sandia National Laboratory*	Analysis of the Heyd-Scuseria-Ernzerhof Density Functional Parameter Space	poster
#79 J. Nicklas *Ohio State University*	Hybrid Density Functional Study of the Electronic Properties for (Hg,Cd)Te Systems	
#80 T. Olsen *Technical University of Denmark*	Accurate Correlation Energies from a Renormalized Adiabatic Local Density Approximation	poster

#81 H. Park *Ohio State University*	Accurate Computational Studies of Carbon Doped Two-Dimensional Boron Nitride	poster
#82 K. Park *Virginia Tech*	Stability of Surface States of Topological Insulators upon Nonmagnetic Absorption	
#83 F. Petruzielo *Cornell University*	Semistochastic Projection	
#84 A. Punya *Case Western Reserve University*	Valence Band Effective Hamiltonians in Nitride Semiconductors from QSGW Band Structures	poster
#85 W. Purwanto *College of William and Mary*	Efficient, Pseudopotential-Free Auxiliary-Field Quantum Monte Carlo Calculations in Solids	poster
#86 Y. Quan *University of California Davis*	Formal Valence, d Occupation, and Charge-Order Transitions	
#87 T. Rawal *University of Central Florida*	Electronic and Optical Properties of Benzylpiperazine/CuI (111) System	poster
#88 W. Ruan *Georgia Institute of Technology*	Graphene Nanoribbons with a Magnetic Edge	poster
#89 D. Saldana-Greco *University of Pennsylvania*	Thermodynamic Stability of the CaMnO3 (001) Surface	poster
#90 G. Samsonidze *Robert Bosch LLC*	Transport Properties of Thermoelectric Materials from First Principles	
#91 K. Schwarz *Cornell University*	Coupled Cluster Studies of Molecules in Condensed Matter Environments	
#92 S. Shah *University of Central Florida*	Self-Diffusion of Ag, Cu, and Ni Islands on Surfaces: An Application of SLKMC-II	poster
#93 B. Shih *State University of New York at Buffalo*	Screened Coulomb and Exchange Parameters of Localized Electrons in the Self-Consistent Constrained RPA	
#94 A. Singh *Cornell University*	Molecular Dynamics Study of Ripples in Graphene and Bilayer Graphene	poster
#95 R. Sundararaman *Cornell University*	A Framework to Generalize Polarizable Continuum Models to Capture the Non-Local Dielectric Response of Solvents (grad student prize)	poster
#96 M. Taherinejad *Rutgers University*	Bloch-type Ferroelectric Domain Walls in Rhombohedral BaTiO3 (grad student prize)	poster

#97 Y. Virgus *College of William and Mary*	Many-Body Study of Cobalt Adatoms Adsorbed on Graphene	
#98 A. Wadehra *The Ohio State University*	Hybrid Density Functional Study of 2D Graphene-Boron Nitride Nanostructures (postdoc prize)	poster
#100 L. Wang *Brookhaven National Laboratory*	The Disorder Effects in Ru Substituted BaFe2As2: Realization of Superdiffusion Mechanism	
#101 A. Wysocki *University of Nebraska-Lincoln*	Microscopic Origin of the Structural Phase Transitions at the Cr2O3 (0001) Surface	poster
#102 L. Xian *Georgia Institute of Technology*	Wave Packet Dynamics in Twisted Bilayer Graphene	
#103 J. Yan *Towson University*	Optical Phonon Anomaly in Bilayer Graphene with Ultrahigh Carrier Densities	poster
#104 H. Zhuang *Cornell University*	Optical Properties of Twisted Bilayer Graphene	
#C J. Shepherd *University of Cambridge, UK*	The Homogeneous Electron Gas: Beyond Fixed Nodes	poster
#D S. Liu *University of Pennsylvania*	Development of a Classical Potential for PbTiO3	

List of Participants:

Addagarla, Tejas: University of Massachusetts at Amherst
Aminpour, Maral: University of Central Florida
Baroni, Stefano: SISSA, Trieste, Italy
Bartlett, Rodney J.: University of Florida
Beck, David: Princeton University (Wake Forest University for the summer)
Bennett, Joe: Rutgers University
Berlijn, Tom: Brookhaven National Laboratory
Bernholc, Jerry: NC State University
Birol, Turan: Cornell University
Bowler, David: University College London, England
Cancio, Antonio: Ball State University
Canepa, Pieremanuele: Wake Forest University
Ceperley, David: University of Illinois at Urbana-Champaign
Chan, Garnet: Princeton University
Cheiwchanchamnangij, Tawinan: Case Western Reserve University
Chen, Zuojing: University of Massachusetts at Amherst
Cho, Sam: Wake Forest University
Chou, Mei-Yin: Academia Sinica, Taiwan

Clark, Bryan: Princeton University
Das, Hena: Cornell University
Dogan, Mehmet: Yale University
Dong, Rui: NC State University
Fellinger, Michael: The Ohio State University
Filippi, Claudia: University of Twente, The Netherlands
Garrity, Kevin: Rutgers University
Gavin, Brendan: University of Massachusetts at Amherst
Georgescu, Alexandru Bogdan: Yale University
Ghosh, Saurabh: Cornell University
Goldsmith, Zachary: University of Pennsylvania
Goerling, Andreas: University of Erlangen-Nurnberg, Germany
Gonzalez Hernandez, Rafael: Universidad del Norte, Colombia
Guo, Yuzheng: Cambridge University, England
Han, Chengbo: Center for High Performance Simulation, NC State University
Hodak, Miroslav: NC State University
Holmes, Adam: Cornell University
Holzwarth, Natalie: Wake Forest University
Hong, Sampyo: University of Central Florida
Honrao, Shreyas: Cornell University
Huang, Ling-Yi: Case Western Reserve University
Huang, Shouting: Washington University in St. Louis
Irikura, Karl: NIST
Ismail-Beigi, Sohrab: Yale University
Jiang, Jie: Yale University
Jiang, Lai: University of Pennsylvania
Johnson, Daniel: Wake Forest University
Jurchescu, Oana: Wake Forest University
Kabir, Alamgir: University of Central Florida
Kakekhani, Arvin: Yale University
Kara, Abdelkader: University of Central Florida
Kaur, Amandeep: University of California at Davis
Kent, Paul: Oak Ridge National Laboratory
Kestyn, James: The University of Massachusetts at Amherst
Kim, Jeongnim: Oak Ridge National Laboratory
Kim, Seungchul: University of Pennsylvania
Kolb, Brian: Wake Forest University
Kozinsky, Boris: Bosch Research
Lee, Jeehye: Cornell University
Lepley, Nicholas: Wake Forest University
Letchworth-Weaver, Kendra: Cornell University
Li, Qi: Wake Forest University
Li, Yan: NC State University
Liang, Yufeng: Washington University in St. Louis
Liu, Shi: University of Pennsylvania
Liu, Yuanyue: Rice University

Longo-Pazos, Roberto: University of Texas at Dallas
Lopez, Graham: Wake Forest University
Lopez-Perez, William: Universidad del Norte, Colombia
Lu, Deyu: Brookhaven National Lab
Lu, Wenchang: NC State University
Marom, Noa: UT Austin
Martins, Cyril: CEA, France
Martirez, John Mark: University of Pennsylvania
Marzari, Nicola: EPFL, Switzerland
Matthews, Rick: Wake Forest University
McMahon, Jeff: University of Illinois
McMinis, Jeremy: University of Illinois
Mendez Polanco, Miguel Angel: University of Pennsylvania
Merle, John: Winston Salem State University
Modine, Normand: Sandia National Laboratories
Montgomery, David: Wake Forest University
Moussa, Jonathan: Sandia National Laboratories
Nicklas, Jeremy: The Ohio State University
Olsen, Thomas: Technical University of Denmark
Parker, James: U.S. Army Research Office
Park, Hyoungki: The Ohio State University
Park, Kyungwha: Virginia Tech
Punya, Atchara: Case Western Reserve University
Purwanto, Wirawan: College of William & Mary
Quan, Yundi: University of California at Davis
Quina, Frank: University of Sao Paulo, Brazil
Ranjan, Vivek: NC State University
Rappe, Andrew: University of Pennsylvania
Rawal, Takat: University of Central Florida
Reboredo, Fernando: Oak Ridge National Laboratory
Resta, Raffaele: SISSA, Trieste, Italy
Ruan, Wen Ying: Georgia Institute of Technology
Salam, Akbar: Wake Forest University
Saldana-Greco, Diomedes: University of Pennsylvania
Samsonidze, Georgy: Bosch Research
Schwarz, Kathleen: Cornell University
Shah, Syed Islamuddin: University Of Central Florida
Shepherd, James: University of Cambridge, England
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