TANER YILDIRIM

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RESEARCH INTERESTS

My research addresses structural, magnetic, and transport properties of novel materials with an eye toward practical applications. This is done by calculating the properties of real materials using first-principles computational techniques and testing the results by neutron scattering and other measurements. Systems of particular interest include molecular solids such as the fullerenes and cubane, nanoporous materials such as metal-organic frameworks for hydrogen storage, frustrated magnetic systems such as the Kagome lattice and cuprates, novel superconductors such as iron-pnictides, doped fullerenes and magnesium diboride, and nanomaterials such as graphene, nanotubes and molecular magnets.

PROFESSIONAL EXPERIENCE

- **NIST Fellow: 2010-present**
- **Adjunct Professor: 2006-present**
  Materials Science and Engineering, University of Pennsylvania, PA 19104
- **Computational and Neutron Science Team Leader: 1998-present**
  NIST Center for Neutron Research, Gaithersburg, Maryland 20899-8562.
- **Research Associate: 1994-1998**
  University of Maryland, College Park, Maryland and NCNR, NIST.

EDUCATION

- **PhD 1990-1994** Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania.
  Thesis: Theoretical and experimental study of solid C_{60} and its Na-doped derivatives and also quantum magnetism and magnetic structures of lamellar perovskite antiferromagnets.
  Thesis Advisors: Prof. A. B. Harris and Prof. J. E. Fischer
- **MSc 1988-1990** Department of Physics, Middle East Technical University, Ankara, Turkey.
  Thesis: Electron-phonon interactions in low dimensionally confined quantum well type semi-conductors. Thesis Advisor: Prof. Atilla Ercelebi
- **BS 1985-1988** Department of Physics, Middle East Technical University, Ankara, Turkey.

PUBLICATIONS

- Over 165 peer-reviewed papers in theoretical and experimental physics and materials science
- Over 7500 citations and 100 invited presentations
- **h-factor = 48**
- **Average citation ~ 47.4**

AWARDS

- **2013 Samuel Wesley Stratton Award** "*for the outstanding scientific achievements in the field of iron-based superconductors in support of NIST objectives*"
- **2009 TUBITAK Special Science Award** *Turkey's highest awards for scientific achievement.*
- **2008 APS Fellowship** *"For combining analytic theory, first-principles computations, and neutron scattering measurements to design, discover, and understand new materials with novel physics."*
- **2007 Arthur S. Flemming Award** *"For outstanding accomplishments in investigations of the properties of novel superconductors and hydrogen storage materials using neutron scattering experiments and associated first-principles calculations".*
- **2007 United States, Department of Commerce, Gold Medal** Award "*For scientific breakthroughs in the creation and characterization of nano-structured materials for safe and efficient solid-state hydrogen storage*"
- **2006 Neutron Scattering Society of America (NSSA) Science Prize** "*For innovative coupling of first-principles theory with neutron scattering to solve critical problems in materials science*"
- **2004 United States, Department of Commerce, Bronze Medal** Award "*For seminal research on creating nanodevices by tuning the properties of carbon nanotubes*"
- **2002 NIST Sigma Xi Award** for Outstanding Young Scientist.
- **1993 Materials Research Society Award** for *recognition of outstanding performance in the conduct of research*

GRANTS

- **2008-2013** Department of Energy BES Grant on *From Fundamental Understanding to Predicting New Nanomaterials for High-Capacity Hydrogen Storage*. $900,000/3 years
- **2005-2010** NIST Innovations in Measurement Science (IMS) Grant *on Fundamental Metrology for Carbon Nanotube Science and Technology*, a collaborative research between Polymer, Optical Technology, Ceramics, Mat. Reliability, and NCNR (Dr. Yildirim).
- **2005-2008** Department of Energy EERE Grant on *Carbide-Drived Carbons with Tunable Porosity Optimized for Hydrogen Storage*, a collaborative research:UPenn, Drexel, and NIST.
- **2001-2003** National Science Foundation Grant No: INT 01-15021: *Experimental and Theoretical Investigation of Nanoscale Materials and Devices Based on Carbon Nanotubes*, a collaborative research project: University of Pennsylvania, NIST, and Bilkent University, Ankara, Turkey.
- **1998-2000** National Science Foundation Grant No: INT 97-31014: *International Cooperative Research Project on Cubane: Univ. of Maryland, NIST, and Bilkent University, Ankara, Turkey.*

RECENT SCIENTIFIC ACTIVITIES

- Served as an DOE EFRC Panelists for Science Reviews - January 25 and 26, 2012 - Denver, CO
- Organized a session on "Advanced Materials for Energy Applications" for the American Crystallographic Association (ACA) meeting, Chicago, 2010.
- Served as a panel member at the DOE Workshop on "Carbon Capture; Beyond 2020", March, 2010.
- Organized focused sessions on "Hydrogen Storage" for the Division of Materials Physics, APS March Meeting, 2007.

- Co-organizer for the summer school "Representational Analysis of Complex Magnetic Structures", July 2007 (http://www.ncnr.nist.gov/staff/taner/racmagstr)
- Designed and build several fully computer controlled high-pressure state-of-the-art Sievert apparatus for hydrogen storage study at NCNR, 2007
- 2006-Present Member of Science Panel, Turkish NanoScience and Technology Center (UNAM).
- Organized an international summer school on "Quantum Computation at the Atomic Scale: QCAS2003", June 1-11, 2003, Istanbul, Turkey. For more information, see the website: http://www.ncnr.nist.gov/staff/taner/workshop/qcas2003
- Organized an international workshop on "Theory, Modeling, and Neutron Scattering; TMNS03", Aug. 12-14, 2003, NCNR, Gaithersburg, MD. For more information see the website: http://www.ncnr.nist.gov/staff/taner/workshop/tmns03
- Build and maintain two state-of-the-art diskless infiniband Beowulf clusters of 96 and 64 nodes for high performance computing at NCNR.
- Organizer, focused sessions on Fullerenes and Nanotubes for the Division of Materials Physics, APS March Meeting, 2001.

PROFESSIONAL MEMBERSHIPS

- American Physical Society Fellow (APS),
- Neutron Scattering Society of America (NSSA)
- NIST Chapter Sigma Xi Scientific Research Society
- American Chemical Society (ACS)
- American Crystallography Association (ACA)

CURRENT and FORMER POSTDOCS

- Dr. Yang Peng and Vaiva Krungleviciute (PENN, 2012-Present).
- Dr. Xuhui Luo (a joint postdoc with Prof. Serdar Ogut, UIC, 2011-2012)
- Jacob Burres, Jamie Ford and Srinivas Gadipelli (UPENN, 2010-2012).
- Dr. Jason Simmon (2008-2010)
- Dr. Wei Zhou (2006-2008)
- Dr. Jorge Iniguez (2003-2005)
- Dr. Oguz Gulseren (2001-2003)

MAJOR ACCOMPLISHMENTS

- ***Phonon-driven superconductivity in the vicinity of ferroelectric and charge density wave ordering in La(O,F)BiS$_2$*** Very recently a new family of layered materials containing BiS_2 planes was discovered to be superconducting at temperatures up to 10 K. These new systems $REO_xF_{1-x}BiS_2$ (RE=La, Nd, Pr, and Ce) are structurally similar to the layered, iron-based superconductors $LaO_xF_{1-x}FeAs$, and in both cases the superconductivity is achieved by F-doping. In addition, band structure calculations indicate the presence of strong Fermi surface nesting at the wave vector (π,π), which is the hallmark property of the Fe-pnictides. These similarities have raised the exciting question of whether or not the superconducting mechanism in the BiS_2 system is related to that in the iron pnictides or cuprates and have therefore generated enormous interest. The fundamental question is whether or not the observed T_c in this new system can be understood within a conventional electron-phonon coupling framework, or is a more exotic mechanism responsible for the superconducting pairing? In this work (T. Yildirim, **Phys. Rev. B 87,** 020506 **(R)**, (2013)) we performed state-of-the-art first principles calculations that directly address this

question and reveal several surprising findings. We show that the parent compound $LaOBiS_2$ possesses highly anharmonic, ferroelectric, soft phonons at the zone center and a spontaneous polarization of ~10 $\mu C/cm^2$ that is comparable to that in the well-known multiferroic $BiFeO_3$. Upon electron doping new instabilities appear at ($\pi/2,\pi/2$) and (π,π), which causes the Bi/S atoms to order into a one-dimensional charge density wave (CDW). We find that BiS_2 is a strong electron-phonon coupled superconductor in close proximity to competing ferroelectric and CDW phases. Our results suggest new directions with which to tune the balance between these phases and increase T_c in this new class of materials. The results reported here bring us much closer to understanding the mechanism of superconductivity in the newly discovered BiS_2 based superconductors and represent a significant contribution to the field of superconductivity, one of the most studied and fascinating areas in condensed matter physics.

- **Methane Storage in Metal–Organic Frameworks: Current Records, Surprise Findings, and Challenges** The research area of methane storage in MOFs has really taken off in the past year or so on account of success here in the U.S. in economically accessing enormous amounts of natural gas trapped in deep shale deposits. There is an almost unbelievable boom in North America, with energy imports dropping hugely, and the price of natural gas decreasing by ~70% since 2008. As vehicle fuel, natural gas is now significantly cheaper here than petrol. This development, along with the widespread opinion that natural gas is a bridging fuel that will supplant coal and oil until renewables are fully in place, has brought research on porous materials for natural gas storage sharply into focus at the U.S. Dept. of Energy. Very recently DOE promulgated new targets for gravimetric and volumetric storage and then followed up with tens of millions of dollars in new, competitively awarded funding to go after the problem. With these new targets, now is an opportune time to evaluate the most promising existing MOFs at pressures higher than 35 bar (the upper bound of most previous studies) and to assess gravimetric uptake, which has not usually been considered in earlier studies. Also important to consider are distinctions between excess uptake, total uptake, and working capacity (deliverable capacity). Re-evaluation also provides an opportunity to: a) take advantage of advances in MOF synthesis and activation that may yield larger surface areas and pore volumes than previously obtained, b) benchmark experimental surface areas against computationally estimated maximum values, and c) standardize comparisons to a specific experimental temperature (298K). Hence, to yield the most consistent and useful experimental benchmarks for studies going forward, it is important to compare data obtained by the same experimentalists and on the same volumetric Sievert apparatus. Herein (**J. Am. Chem. Soc. 135**, 11887-11894 (2013)) we report such a study. Perhaps our most surprising finding is that HKUST-1, a MOF that is available commercially in gram scale, exhibits the highest total, ambient temperature, volumetric uptake of CH_4 of any MOF reported thus far. The value for HKUST-1 at 65 bar and 298 is 267 cc(STP)/cc, on par with a CNG tank at 255 bar. With these results in mind, we additionally examined how MOF packing density relates to experimentally obtainable volumetric working capacity, and how intentional MOF compaction and wafer formation influence both volumetric and gravimetric working capacities. These considerations are likely to lead to a re-ordering of MOF performance rankings and underscore the need to move toward materials that are efficiently packable, yet capable of withstanding mechanical compression and retaining full sorption capacity. With the most promising existing MOFs now uniformly experimentally evaluated on an applications-relevant basis, we anticipate that the results of future investigations with new materials and/or processing techniques will be straightforward to compare against these benchmark findings. Our strong belief is that our work will prove to be a gold standard study against which nearly all other studies for the next four or five years will seek to compare.
- **Efficient Carbon Capture in Metal-Organic Frameworks (MOFs).** Carbon capture is a critical component of the mitigation of CO_2 emissions from industrial plants. Investigations of the application of MOFs to adsorptive carbon capture have focused on their appreciable storage capacities but fail to address the more pertinent issue of how MOFs perform under common industrial separation processes that are at the heart of carbon capture. Typical processes rely on swing adsorption and are limited to relatively low CO_2 partial pressures such that the total pore volume and the surface area are under-utilized. Here (**Energy Environ. Sci. 4, 2177 (2011)),** we investigate the performance of a number of metal–organic frameworks with particular focus on their behavior at the low pressures commonly used in

swing adsorption. This comparison clearly shows that it is the process that determines which MOF is optimal rather than there being one best MOF, though MOFs that possess enhanced binding at open metal sites generally perform better than those with high surface area. This work will be an important guideline for deciding the best pair of carbon capture process and MOF material for optimum carbon capture.

- ***Graphene Oxide Framework Materials Suggested for Hydrogen Storage and Carbon Capture***: In this study, we show that one-and-a-half-century-old graphene oxide (GO) can be easily turned into a potentially useful gas storage material. GO is a sheet of carbon atoms with many hydroxyl, epoxide and carboxyl surface groups. In principle, hydrogen can be stored between layers of this lightweight material. However, the challenge is to separate the layers without filling the space between them. Here we show that by using the well-known chemistry between diboronic acids and hydroxyl groups, GO layers can be linked together to form a new layered structure. Such GOF structures have tunable pore widths, volumes, and binding sites depending on the linkers chosen, and could exhibit interesting gas sorption properties. As discussed in the manuscript, ideal GOF structures can adsorb hydrogen up to 6 wt% at 77 K and 1 bar, a value higher than any other porous material known. Our synthesized GOF materials exhibit 9 kJ/mol and 32 kJ/mol isosteric heat of adsorption for H2 and CO2, significantly larger than those found in similar nanoporous materials. The nitrogen BET surface area reaches a maximum at 470 m2/g. Despite this low surface area, GOF exhibits 1 wt% H2 uptake at 1 bar. This is much less than what the 'ideal' GOF structure can hold, suggesting that our initial synthesized GOF materials could be significantly optimized in the near future. For details, see "Graphene Oxide Framework Materials: Theoretical Predictions and Experimental Results", Angew. Chem. Int. Ed. 2010, 49, 8902-8904.

- ***Competing Magnetic Interactions, Structural Phase Transition, and the Key Role of the Fe-spin State in Iron-Pnictide Superconductors:*** We have performed several important studies on various iron-pnictide systems from first-principles and neutron scattering measurements. In particular, for the first-time, we have shown that there are strong competing antiferromagnetic interactions in FeAs plane, suggesting magnetism and superconductivity in doped LaOFeAs may be strongly coupled, much like in the high-T_c cuprates[T. Yildirim, Phys. Rev. Lett. **101**, 057010 (2008)]. From accurate all-electron fixed-spin-moment calculations, we clearly showed that the ferromagnetic and checkerboard antiferromagnetic ordering in LaOFeAs were not stable and the stripe antiferromagnetic Fe-spin configuration (i.e. SDW) was the only stable ground state. We further showed that the main exchange interaction between Fe ions are large, antiferromagnetic, and frustrated. We found that only the magnetic stripe SDW phase breaks the tetragonal symmetry, removes the frustration, and causes a structural distortion. We even predicted several fine-details of the magnetic structure such as the ferromagnetically alinged spin direction in SDW state is along the short axis. This prediction has been now confirmed in several 122 systems (i.e. $SrFe_2As_2$) from single crystal neutron data. In support of the important role of Fe-magnetism in these systems, very recently we showed that Fe-spin state in iron-pnictides has an unprecedented control on the structural and other physical properties of these systems. We discovered surprisingly strong interactions between arsenic ions, the strength of which is controlled by the Fe-spin state in an unprecedented way. Reducing the Fe-magnetic moment, weakens the Fe-As bonding, and in turn, increases both intra-and inter-plane As-As interactions, causing giant reduction in the c-axis. For $CaFe_2As_2$ system, this reduction of c-axis with the loss of the Fe-moment is as large as 1.4 Å, an unheard of giant coupling of local spin-state of an ion to its lattice. Since the calculated large c-reduction has been recently observed only under high-pressure, we suggest that the iron magnetic moment should be present in Fe-Pnictides at all times at ambient pressure. The giant coupling of the on-site Fe-magnetic moment with the As-As bonding that we have discovered in Ref.[T. Yildirim, PRL **102**, 037003 (2009):arXiv:0807.3936v2] may provide a mechanism for the superconductivity.

- **Metal-Organic Molecule Complexes as a high-capacity hydrogen storage medium** We have recently predicted (**Phys. Rev. Lett. 97, 226102 (2006)**) that a single ethylene molecule can form stable complexes with light transition metals (TM) such as Ti and the resulting TM-ethylene complex can

absorb up to 12 and 14 wt % hydrogen for n=1 and 2, respectively. Extending this study to include a large number of other metals and different isomeric structures yielded interesting results for light metals such as Li. The ethylene molecule is able to complex with two Li atoms with a binding energy of 0.7 eV/Li which then binds up to two H2 molecules per Li with a binding energy of 0.24 eV/H2 and absorption capacity of 16 wt %, a record high value reported so far. The stability of the proposed metal-ethylene complexes was tested by extensive calculations such as normal-mode analysis, finite temperature first-principles molecular dynamics (MD) simulations, and reaction path calculations. The phonon and MD simulations indicate that the proposed structures are stable up to 500 K. The reaction path calculations indicate about 1 eV activation barrier for the TM_2-ethylene complex to transform into a possible lower energy configuration where the ethylene molecule is dissociated. Importantly, no matter which isometric configuration the TM_2-ethylene complex possesses, the TM atoms are able to bind multiple hydrogen molecules with suitable binding energy for room temperature storage. These results suggest that co-deposition of ethylene with a suitable precursor of TM or Li into nanopores of light-weight host materials may be a very promising route to discovering new materials with high-capacity hydrogen absorption properties. Interestingly, an independent group at University of Virginia have recently confirmed our predictions by demonstrating about 14 wt% H2 absorption on a thin-film of Ti-C2H4 complex at room temperature (see Phys. Rev. Lett. **100**, 105505 (2008)).

- ***Packing Hydrogen into Three Dimensional Networks of Nano-Clusters*** The success of future hydrogen and fuel-cell technologies is critically dependent upon the discovery of new materials that can store large amount of hydrogen at ambient conditions. Metal-organic framework (MOF) compounds, which consist of metal-oxide clusters connected by organic linkers, are a relatively new class of nano-porous material that show promise for hydrogen storage applications because of their tunable pore size and functionality. In this letter (**PRL Nov.23 issue 2005**), using difference-Fourier analysis of neutron powder diffraction data along with first-principles total-energy calculations, for the first time, we directly determine the available adsorption sites in MOF5. Surprisingly, the MOF5 host lattice has enough space available to hold many hydrogen molecules, up to ~10 wt-% at low temperatures. We determined the nature of the MOF-hydrogen interaction and the manner in which hydrogen molecules are adsorbed onto the structure. These results hold the key to engineering MOF materials for practical hydrogen storage applications. Equally important, we find that at high-concentration loadings hydrogen molecules form unique 3 dimensional networks of H_2 nano-clusters with short intermolecular distances. These findings suggest that MOF materials can also be used as templates to create artificial, interlinked hydrogen nano-cages. Such materials could exhibit very unexpected properties due to quantum confinement effects and the small intermolecular distances, such as metallic behavior. More information about this work can be obtained at http://www.ncnr.nist.gov/staff/taner/h2

- ***Ti-decorated Nanostructures as a Potential High Capacity Hydrogen Storage Medium*** Recently much effort has been focused on the search of new routes to engineer nanomaterials so that they dissociate H_2 molecules into H atoms and reversibly adsorb hydrogen molecules at ambient conditions. It is found that while hydrogen-carbon interaction is too weak, the metal-hydrogen interaction is too strong for room temperature reversible storage. In this work (**PRL 94, 175501**) we show a novel way to overcome this difficulty by forming artificial metal-carbides on nanotubes fullerens! Our accurate quantum mechanical calculations show that a single Ti-atom coated on a SWNT/C_{60} can strongly adsorb up to four hydrogen molecules. The hydrogen-metal bonding is an unusual combination of chemi- and physi-sorption, an essential ingredient needed for reversible hydrogen storage medium near room temperature. Remarkably, this adsorption occurs with no energy barrier. At large Ti coverage we show that a (8,0) SWNT can store hydrogen molecules up to 8-wt%, exceeding the minimum requirement of 6-wt% for practical applications. Finally, we present high temperature quantum molecular dynamics simulations showing that these systems are stable and indeed exhibit associative desorption of H_2 upon heating, another requirement for reversible storage. These results advance our fundamental understanding of dissociative and molecular chemisorptions of hydrogen in nanostructures and suggest a possible method

of engineering new nanostructures for high-capacity storage and catalyst materials. More information such as animation of the reaction paths and MD trajectories can be found at http://www.ncnr.nist.gov/staff/taner/h2

- ***Magnetically Driven Ferroelectric Order in $Ni_3V_2O_8$*** In recent years there has been marked interest in investigating systems exhibiting simultaneous long range magnetic and ferroelectric orders. The magnetoelectric effects in these multiferroic materials offer insight into the role of spin-charge-lattice couplings in producing complex long-range orders. Developing insulating materials in which charge and spin are strongly coupled may allow the fabrication of new devices incorporating the best of both worlds such as voltage-driven fast switching magnetic memory. However, to date, there has been little understanding of how this multiferroic behavior arises. In this work (**PRL 95, 87205 and PRL 93 247201**), we discuss our measurements on $Ni_3V_2O_8$ and present a model which fully accounts for the observed multiferroic behavior of this material. Our investigations of $Ni_3V_2O_8$, a compound with both charge and spin ordering, are used to develop a model explaining in detail how this spin-charge coupling arises. Understanding this coupling is crucial for developing the materials which will form the basis for future electronic devices. For the first time we presents the discussion of how a ferroelectric phase transition can be driven solely by magnetic order. By carefully investigating the magnetic and ferroelectric properties of $Ni_3V_2O_8$, we have identified a mechanism through which two distinct magnetic order parameters can combine to break the spatial inversion symmetry, which promotes ferroelectric ordering. We believe that $Ni_3V_2O_8$ exhibits an experimental realization of this effect, and are successfully able to explain its novel magnetoelectric couplings. In particular, using solely the symmetries of the magnetically ordered phases, we are able to understand how ferroelectric order in the system can be reversibly switched on and off by applying a magnetic field. The general model we propose is expected to be relevant to understanding a wide range of magnetoelectric multiferroics, and more generally, how complex order parameters can be combined to break symmetries which in turn allows new phases to arise.

- ***Hidden Symmetries and Their Consequences in the t_{2g} Cubic Perovskites.*** In this work (Phys. Rev. Lett, **91**, 087206 (2003) and Phys. Rev. B **69**, 035107 (2004)) we report crucial new results concerning the possible ordered phases *of transition metal perovskites*, and their possible theoretical origins. The transition metal oxides are very important materials, because they have been a rich source of novel and intriguing physical phenomena such as high T_c superconductivity, colossal magnetoresistance (CMR), and most recently, the fascinating *combined spin-orbital ordering phenomena.* Much of the theoretical literature on these systems has used the standard Hubbard model, or its low temperature version derived by Kugel and Khomskii (KK). In this work, for the first time, we show that for the t_{2g} orthogonal perovskites, these models possess several *hidden novel symmetries*, upon which rigorous conclusions can be based. In particular, we use these symmetries to prove that – contrary to the general belief in the literature - these basic models *forbid any long range spin order* at nonzero temperatures. Inclusion of spin-orbit coupling allows such ordering, but even then *the excitation spectrum is gapless* due to a continuous symmetry. Experimental systems, such as $LaTiO_3$, do exhibit long-range order and an excitation spectrum with a gap. The important point of our work is that we show that a consistent theoretical explanation of such experimental facts *must* include additional suitable *perturbations to the Hubbard or to the KK Hamiltonian*. We also show that the uncovered symmetries of the Hubbard model are very useful in *exact numerical studies of finite clusters*. For example, finding the ground state of a cube of eight Ti ions requires the diagonalization of a matrix having *about ½ million rows and columns*. However, using the symmetries discovered in this Letter, this problem is reduced to a *16x16* dimensional matrix diagonalization! It is surprising that, although the crystal field theory of cubic perovskites and the corresponding Hubbard model have been the subjects of many studies and even textbooks, the novel hidden symmetries uncovered in this work were still missed. Hence, we expect that this work will make a big impact in the physics community and that these results will inspire experimentalists to synthesize new t_{2g} transition metal oxides with tetragonal or higher symmetry. Such systems would have quite striking and anomalous properties.

- ***Theory of Superconducivity in MgB_2.*** The surprising discovery of superconductivity in magnesium diboride (MgB_2) at 39 K raised the question of whether the origin of the high T_c is due to electron-phonon coupling as is the case for "conventional" superconductors or to a more exotic mechanism. By combining first-principles calculations and inelastic neutron scattering measurements of the phonons in MgB_2, we demonstrated that the in-plane boron phonons (with E_{2g} symmetry) near the zone-center are very anharmonic. Moreover our calculations revealed that these modes strongly couple to the partially occupied planar B σ electronic bands near the Fermi level. We showed that this giant anharmonicity and non-linear electron-phonon coupling is the key to quantitatively explaining not only the observed high T_c and boron isotope effect in MgB_2 but also the pressure dependence of the T_c. This work (Phys. Rev. Lett. **87**, 37001 (2001)) has received a great deal of interest within the physics community as evidenced by articles in Physical Review Focus (July 2001) and in the September 2001 issue of Materials Today.

- ***First Principles Calculations of Carbon Nanotubes.*** Carbon nanotubes, originally discovered as a by-product of fullerenes synthesis, are one of the most promising nanomaterials. We have used first principles calculations to elucidate details of the electronic and chemical properties of these systems. Our first work in this area resulted in the prediction that by applying pressure, carbon nanotubes can be covalently joined to form one and two-dimensional networks of interlinked nanotubes (Phys. Rev. B **62**, 12648 (2000)). Several months after our prediction was published, the results were independently confirmed experimentally (see Phys. Rev. Lett. **86**, 3056 and Phys. Rev. B **64**,153401). The second major accomplishment in nanotube research was the discovery that the band gap of an insulating nanotube can be engineered by elliptical distortion (Phys. Rev. B **62**, R16345 (2000)). This work has significant implications for designing electronic nanodevices based on nanotubes. Finally, we have very recently shown (see Phys. Rev. Lett. **87**, 116802 (2001)) that the chemical reactivity of nanotubes can be tuned by elliptical deformation, which may provide a way to attach various atoms such as metals to a specific location on a nanotube. An article about our research appeared in the November issue of Materials Today 2000. Further details of this research can be found at http://www.ncnr.nist.gov/staff/taner/nanotube.

- ***The Structure and Dynamics of Solid Cubane.*** The cubane molecule (C_8H_8) is aesthetically appealing due to the highly symmetric cubic shape. Moreover it is the most highly strained, kinetically stable ring system available in quantity, and therefore offers promise in many diverse and interesting practical applications as explosives, high-refractive index lenses, specialty polymers, and fuel additives. While cubane was first synthesized and the room temperature crystal structure was determined in the early 1960's, the high temperature, orientation ally disordered structure remained unknown due to experimental difficulties arising from the high vapor pressure and the associated problem of recrystallization. In 1997, we surmounted these challenges and using X-ray and neutron scattering along with various theoretical models, characterized the disordered phase of solid cubane (see Phys. Rev. Lett. **78,** 4938 (1997)). This work received enormous interest as evidenced by articles in The New York Times (July 15, 1997), Science News (**52**, p. 34, 1997), and Physics Today News Updates (p. 9 August 1997). More recently, a review of our work on cubane appeared in Neutron News (**12**, No.2, p. 34 (2001)).

- ***The Synthesis and Characterization of Na_xC_{60}.*** The discovery of a simple method of making large quantities of fullerenes initiated a great deal of research into the properties of fullerenes and compounds based on fullerenes. Several phases of C_{60} with alkali metals such as K, Rb, and Cs were reported. However, due to reactivity of smaller alkali metals and several þechnical difficulties, the phase diagram of C_{60} with Na and Li were not known. In 1992 we developed a new synthesis technique using copper tubing and alkali-metal azide to remedy these difficulties and reported the first solid-state synthesis and x-ray characterization of the saturated phase of the Na-C_{60} system (Nature **350**, 568 (1992)). This work

suggested that by using smaller alkali metals (*i.e.*, Li), it would be possible to intercalate even more atoms into the host lattice, a finding of great interest for Li batteries.

- ***Theory of Orientational Ordering in C_{60} and C_{60}-based Compounds*.** C_{60} molecules adopt several different orientations in the solid state depending on various factors including temperature and intercalated species. In 1993, we combined synthesis and characterization of new C_{60} based materials with theoretical calculations to provide a unified view of orientational ordering of C_{60} in C_{60}-based solids (Phys. Rev. Lett. **71**, 1383 (1993)). This work resulted in the widespread realization of the importance of molecular orientational order/disorder phenomena on properties such as superconductivity.

- ***The Role of Carrier Concentration in Superconductivity of C_{60}-based Compounds***. The discovery of superconductivity in A_3C_{60} compounds where A is K, Rb, or Cs sparked a great deal of interest in the condensed matter physics community. It was quickly realized that the superconducting transition temperature depends strongly on the lattice constant which could be easily controlled by changing the alkali metal or by applying external pressure. This dependence was attributed to the changing density of electronic states at the Fermi level. To explore this idea further, one would like to adjust the carrier concentration in these systems. Unfortunately this is fixed at three electrons per C_{60} molecule due the narrow solubility range in the phase diagram of these compounds. We overcame this problem by synthesizing two novel families of fullerides, $Na_2Cs_xC_{60}$ and $M_{3-x}Ba_x\ C_{60}$, thereby allowing the first studies of the correlation between the superconducting transition temperature and the carrier concentration. (Phys. Rev. Lett. **77**, 167 (1996)). This work clearly demonstrated that the mechanism of superconductivity in these systems is unique and quite different than that in the high T_c cuprates.

- ***Theory of Spin Orbit Interactions and Magnetic Anisotropy in Magnetic Insulators*.** A longstanding problem concerns the mechanism whereby spin-orbit interactions give rise to magnetic anisotropy in magnetic insulators. Until recently the discussions of the origins of anisotropy found in cuprates were confined to the orthorhombic structure (*i.e.*, La_2CuO_4) However, more recently a family of copper oxide materials of similar structure, but which are actually tetragonal, have been studied and found to have roughly the same out-of-plane anisotropy as La_2CuO_4. The earlier studied did not predict any anisotropy in the tetragonal limit. Explaining this discrepancy was the main purpose of our work. We developed a theory which for the first time corrects, extends, and clarifies results concerning the spin Hamiltonian used to describe the ground manifold of Hubbard models for magnetic insulators in the presence of spin-orbit interactions. (Phys. Rev. Lett. **73**, 2919 (1994)). The biggest impact of this work is the demonstration that the orthorhombic distortion is not responsible for the observed anisotropy of the spin structure in the cuprates. Rather our theory shows that this anisotropy is due to spin-orbit and Coulomb exchange interactions.

PUBLICATIONS

1. "*Relationship between Se height and spin configuration of the underlying Fe square and the formation of Fe vacancies in* $M_xFe_{2-y}Se_2$", Xuhui Luo, S. Ogut, and T. Yildirim, **Phys. Rev. B** (in review, 2013).

2. "*A Robust N-rich Porous Organic Framework for* CO_2 *Capture and Separation*" M. Das, J.B. Lin, W, Zhou, Taner Yildirim, G. Shimizu, **Chem. Materials** (in review, 2013).

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INVITED TALKS

1. *Methane Storage in Metal-Organig-Frameworks* invited talk at the 246th ACS Fall Meeting, Indianapolis, IN, September, 2013.
2. *From fundamental understanding to predicting new nanomaterials for high capacity hydrogen and methane storage*, Seminar at Northwestern University, Evanston, IL (host: Joe Hupp/Omar Farha), June 2013.
3. *Methane Storage in Metal–Organic Frameworks: Current Records, Surprise Findings, and Challenges*, invited talk at the ACS Spring Meeting, New Orleans, LA, April 2013.
4. *Boron based Materials for Hydrogen Storage*, invited talk at MS&T'12, Pittsburg, Pennsylvania, October 2012.
5. *From fundamental understanding to predicting new nanomaterials for high capacity hydrogen/methane storage and carbon capture*, Seminar at UNIST, S. Korea, Nov. 2012.
6. *Efficient Carbon Capture in Metal-Organig-Frameworks and Graphene Oxide Derived Carbons*, invited talk at the KAIST Workshop on Carbon Capture, Kaist, S. Korea, Nov. 2012.
7. *Graphene Oxide Derived Carbons (GODC); High-Surface Area NanoPorous Materials for Hydrogen Storage and Carbon Capture*, invited talk at the APS March Meeting, Boston, MA, March 2012.
8. *Efficient Carbon Capture in Metal-Organic Frameworks*, invited talk at the ACS Spring Meeting, San Diego, CA, March 2012.
9. *From Fundamental Understanding to Predicting New Nanomaterials for Methane Storage and Carbon Capture*, invited talk at the DOE MSED Neutron Scattering Meeting, Gaithersburg, MD, July. 2012.
10. *Porous Graphene Oxide Frameworks (GOFs); Synthesis and Gas Adsorption Properties***,** ACS Fall Meeting, Philadelphia, PA, August 2012.
11. *Nanoporous Carbons Derived From Graphene Oxide (GO) and Metal-Organic-Frameworks (MOFs)*, ACS Fall Meeting, Philadelphia, PA, August 2012.
12. *Unraveling secrets of advanced materials through first-principles computation, theory and neutron scattering; the first step towards "Materials Genome"*, Colloquium, MSE, University of Pennsylvania, Philadelphia, PA, October 2011 (Host: Chair Peter Davies).
13. *Boron Based Materials for Hydrogen Storage*, invited talk at 17th International Symposium on Boron, Borides and Related Materials, September 11–17, 2011, Istanbul, Turkey.
14. *Finite-Displacement First-Principles Approach for Understanding Recent Novel Superconductors: from Fe-Pnictides to molecular Picene*", invited talk at "Superconductivity 100 Years Later, a Computational Approach", sponsored by the European Science Foundation, PSIK and CECAM, Alghero, Sardinia, Italy, September 2011.
15. *First-principles investigation of recent novel superconductors: Fe-pnictides and K-doped Picene*, Condensed Matter Colloquium at the Center for Nanophysics and Advanced Materials (CNAM), University of Maryland, Feb. 2011 (host: Prof. Johnpierre Paglione)

16. *From Fundamental Understanding to Predicting New Nanomaterials for High-Capacity Hydrogen*, DOE BES Neutron Scattering Contractors Meeting, Airlie Conference Center, Warrenton, VA, July 2010.

17. *Nanoporous Framework Materials for Hydrogen Storage and Carbon Capture Applications***,** Turkish National Conference On Nano-Science and Technology (NanoTR-VI), Izmirl,Turkey, June, 2010.

18. *Phonons, Spin-waves and Magnetoelectric Interactions in magnetically-driven ferroelectric system $Ni_3V_2O_8$; Towards a Microscopic Model*, invited talk at the CECEM Workshop on Theory of Magnetoelectrics: Fundamentals and Applications, May 2010, Lausanne, Switzerland.

19. *"Key Role of Iron-Magnetism in High-Temperature Fe-Pnictide Superconductors",* colloquium at the Institute for Quantum Matter, Johns Hopkins University, April 2010 (host: Prof. Collin Broholm).

20. *Magnetic and Structural Properties of Fe-pnictide superconductors*, at the international workshop on the new iron-arsenic based superconductors and related materials (IRiSes2009), 25 January 2009 in Ueno (Tokyo), Japan (see http://nsrc.tokai-sc.jaea.go.jp/irises/).

21. *Combined first-principles and neutron scattering study of Fe-pnictide superconductors*, at the 2009 March Meeting of the American Physical Society, March 16-20 in Pittsburgh, Pennsylvania.

22. *Molecular Hydrogen in Nanoporous Materials: Meeting Ground for Theory and Experiment*, invited talk at the ACS symposium, Salt Lake City, Utah, March 22-26, 2009.

23. *Competing Magnetic Interactions and Structural Phase Transition in Fe-pnictide Superconductors*, invited talk at the 2009 American Crystallography Assoc. meeting in Toronto (July 25-29).

24. *Hydrogen Absorption Properties of Metal-Organic-Framework Materials (MOF)*, colloquium at the Physics Department, Miami University, Oxford OHIO, April 16, 2008 (Host: Prof. Hong-Cai Zhou).

25. *Recent Progresses in Hydrogen Storage Research*, the 10th Electric Power Conference (a nation-wide conference held annually (4400 attendance)), Baltimore, Maryland, May 2008.

26. *Engineered Nan-Materials for High-Capacity Hydrogen Storage*, Turkish National Conference On Nano-Science and Technology (NanoTR-IV), ITU, Istanbul,Turkey, June 9-13, 2008

27. *Towards a Microscopic Model of Magnetoelectric Interactions in Multiferroic $M_3V_2O_8$ (M=Ni,Co)*, International Conference On Superconductivity and Magnetism; Antalya-Turkey, August 25-29, 2008.

28. *Engineereed Nanomaterials for High-Capacity Hydrogen Storage*, Colloquim at the Physics Department, University of Illinois at Chicago, Oct. 31, 2007 (Host: Prof. Serdar Ogut).

29. *Computer-Aided Search for Novel Hydrogen Storage Materials*, Computational Materials Science Network (DOE-CMSN) on Surface-Based Nanostructures, Ames Lab, October 5-6, 2007.

30. *Combined first-principles and Neutron Scattering Study of Novel Hydrogen Storage Materials*, International Symposium on "Materials Issues in a Hydrogen Economy", in Richmond, Virginia, November 12-15, 2007.

31. *Computational Studies of Advanced Hydrogen Storage Materials*, invited talk at the XVI International Materials Research Congress, Cancun, MX, Aug. 2007.

32. *Hydrogen in Materials*, invited lecture at the LANSCE "Hydrogen in Materials" Summer School, Los Alamos, July 2007.

33. *Functionalization of carbon based nanostructures with light transition metal atoms for hydrogen storage*, Turkish National Conference On Nano-Science and Technology (NanoTR-III) Bilkent, Ankara, Turkey, June, 2007

34. *Advanced Hydrogen Storage Materials; a first principles and neutron scattering study,* seminar at the Instituto de Ciencia de Materiales de Madrid (Host: Norbet M. Nemes) and Barcelona (Host: Jorge Iniguez), May 2007.

35. *Transition-Metal Organic-Molecule Complexes as high-capacity hydrogen storage medium*, Physics Seminar at the University of Virginia, VA, April 2007 (Host: Prof. Bellave Shivaram).

36. *From fundamental understanding to predicting new materials for high capacity hydrogen storage,* colloquium at the Oak Ridge National Laboratory, TN, Feb. 2007 (Host: David Singh).

37. *Unraveling Secrets of Complex Materials through first-principles computation, theory, and neutron scattering,* ACNS 2006 Science Prize Talk, St. Charles, Illinois, June 2006.

38. *Neutron Scattering and First-Principles Study of Novel Hydrogen Storage Materials*, invited talk at the ACNS 2006 Meeting, St. Charles, Illinois, June 2006

39. *Hydrogen and Methane Storage in Nanocages,* invited talk at the XV International Materials Research Congress, Cancun, MX, Aug. 2006.

40. *Atomic Scale Friction between Boron Nitride Slabs and the Effect of Hydrogenation,* invited talk at the 5th ESF Nanotribology Workshop, Antalya, Turkey, September 2006.

41. *Neutron Scattering and First-Principles Study of Novel Hydrogen Storage Materials*, invited talk at the Materials Research Society, San Francisco, April 2006.

42. *Study of Advanced Hydrogen Storage Materials by Neutron Scattering and Computer*, invited talk at the American Physical Society, Baltimore, March 2006.

43. *Predicting Engineered Nano-materials for High-Capacity Hydrogen Storage*, invited talk at the Materials Research Society, Boston, December 2005.

44. *Predicting Engineered Nanomaterials for Reversible Hydrogen Storage,* at the Materials Science and Engineering Seminar Series, LRSM, University of Pennsylvania, Host: Prof. Jack Fischer, November, 2005.

45. *The Magic Role of Ti in Hydrogen-Storage Materials*, at the Gordon Conference on Hydrogen-Metal Systems, Colby College, Waterville, ME, July 10-15 2005.

46. *Combined first-principles modeling and neutron scattering study of advanced materials*, at the international workshop, Neutrons and Numerical Methods 2, Insitut Lane Langevin, Grenoble, France, September 14-18 2004.

47. Atomic Scale Friction between Hydrogenated Nanostructures and Graphite/Diamond Surfaces, at the 3rd ESF-Nanotribology Workshop, September 2004, Sesimbra, Portugal

48. *Combined neutron scattering and first-principles characterization of hydrogen storage materials,* semi-plenary lecture at the International Symposium on Metal-Hydrogen Systems MH2004, Cracow, Poland, September 5-10 2004.

49. *Neutron Methods for Characterization of Fuel Cell and Hydrogen Storage Materials*, at the JINS workshop on Neutrons & Energy for the Future, Washington DC, June 4-5 2004.

50. *Studying Advanced Materials via Quantum Mechanics and Computers*, at the Institute for Physical Science & Technology, University of Maryland, College Park, Host: Prof. Michael E. Fisher, February 2004.

51. *Prediction and Characterization of Advanced Materials from First-Principles*, at the International Research Workshop of Israel Science Foundation on Transport and Magnetism; From the Thermodynamics Limit to the Nano-Scale, Eilat, Israel, January 2004.

52. *The physical and chemical properties of carbon nanotubes; a first-principles study*, at the condensed matter seminer series, Physics Department, Duke University, Host: Prof. Denis Ullmo, October 30, 2003.

53. *Intimate Relationship between Structural Deformation and Properties of Singe-Walled Carbon Nanotubes and its Hydrogenated Derivatives*, at the NATO-ASI (Advanced Study Institute) on "Nanoengineered Nanofibrous Materials", Antalya Turkey, September 2003.

54. *Quantum Dynamics of H_2 in Nanocages*, at the "International Workshop on the Scientific Opportunities with the Cold Neutron Time-of-Flight Spectroscopy", Bethesda, Maryland, MD, July 2003.

55. *Structural and Electronic Properties of Carbon Nanotubes and Its Derivatives*, at the "Accelrys World Conference", San Diego, CA, February 2003.

56. *Electronic and Structural Properties of 40 K Superconductor MgB_2*, at the Penn State University, University Park, PA 16802 (Host: Prof. Paul Sokol), December 2002.

57. *Hidden Symmetries and Their Consequences in t_{2g} Cubic Perovskites*, at the Physics Department, University of Pennsylvania, Philadelphia, PA (Host: Prof.A.B. Harris), December 2002.

58. *Prediction and Characterization of Materials Properties from First Principles*, at the NIST Sigma Xi Colloquium, November 2002.

59. *The Theory of Superconductivity in MgB_2*, at the First International Workshop on Superconductivity in Magnesium Diboride and Related Materials, Genoa, Italy, June 2002.

60. *First-Principles Calculations and Neutron Scattering*, at the American Conference on Neutron Scattering, Knoxville, TN, June 2002.

61. *First-Principles Study of Structure and Electronic Properties of Carbon Nanotubes*, at the Physics Department, University of Maryland, College Park (Host: Prof. Michael Fuhrer), May 2002.

62. *First-Principles Zone-Center Theory of 40 K BCS Superconductivity in MgB_2*, at the American Physical Society Meeting, Indianapolis, IN, March 2002.

63. *A Simple BCS Theory of 40 K Superconductivity in MgB_2*, at the international symposium on Artificial and Natural Nanostructures - Superstripes, Rome, Italy, December 2001.

64. *First-Principles Calculations for Nanoscale Materials and Devices Based on Carbon Nanotubes*, at a workshop on Computational Nanoscience for Industrial Applications, Houston, TX, October 2001.

65. *Anharmonic Lattice Dynamics and Nonlinear Electron-Phonon Coupling in New 40K Superconductor MgB_2*, at the International Conference on Neutron Scattering (ICNS2001), Munich, Germany (September, 2001).

66. *Experimental and Theoretical Investigation of Nanoscale Materials and Devices Based on Carbon Nanotubes*, at the Applied Statistical Physics Molecular Engineering Conference, Cancun, Mexico, July 2001.

67. *Giant Anharmonicity and Non-Linear Electron-Phonon Coupling in 40 K Superconductor MgB_2*, at the workshop on Spectroscopies of Novel Superconductors, Chicago, IL, May 2001.

68. *New High Tc Boron Superconductor*, at Argonne National Laboratory, Argonne, IL (host: Dr. J.D. Jorgensen) Apri1 2001.

69. *Combined Neutron Scattering and First-Principles Investigation of the New High T_c Boron Superconductor*, at the University of Illinois at Chicago, Chicago, IL (host: Prof. I. Baltra) April 2001.

70. *First-principles and Neutron Scattering Study of Photon Conductors*, at the l0th International Conference on Solid State Protonic Conductors, Montpellier, France, September 2000.

71. *Combined Neutron Scattering and First-Principles Study of Novel Materials*, at the American Crystallographic Association, St. Paul, MN, July 2000.

72. *Structure and Dynamics from First-Principles*, at the MSI Workshop on Applications of Quantum Mechanics in the Catalysis, Chemicals, and Electronic Industries, Chicago, May 2000.

73. *Application of Neutron Scattering Methods to the Study of Protonic Conductors*, at Laboratoire Leon Brillouin, Saclay, France (Host: L.T. Lee) April 2000.

74. *First-principles and Neutron Scattering Study of Structure and Dynamics of Materials*, at Institut Laue-Langevin, Grenoble, France (Host: M. R. Johnson), April 2000.

75. *High-Spin Magnetic Molecules: Molecular Approach to Nanomagnetism*, at the Harris Fest Symposium at the University of Pennsylvania, Philadelphia, PA, March 2000.

76. *Combined neutron scattering and first-principles studies of novel solids*, at the international conference on Neutrons and Numerical Methods, ILL, Grenoble, France, December 1999.

77. *First Principles Calculations and Neutron Scattering*, at the NCNR workshop on Cold Neutron Spectroscopy, Gaithersburg, MD, August 1999.

78. *Carbon Based Molecular Clusters: Cubane and Fullerenes*, at the NATO-ASI meeting NATO on Quantum Mesoscopic Phenomena, Ankara/Antalya, Turkey, June 1999.

79. *First Principles Study of Structure and Dynamics of Solid Cubane*, at the 5th Statistical Physics Meeting, Istanbul Technical University, Turkey, July 1998.

80. *Unusual Structure, Phase Transition, and Dynamics of Solid Cubane*, at the Naval Research Laboratory, Washington, DC (Host: Dr. John Mintmire) June 1998.

81. *Fullerene Based Superconductors*, at the 193th Electrochemical Society Meeting, San Diego, CA, May 1998.

82. *Neutron and X-ray Study of Structure and Dynamics of Solid Cubane*, at the University of North Carolina, Chapel Hill, NC (Host: Prof. Otto Zhou) October 1997.

83. *Unusual Structure, Phase Transition, and Dynamics of Solid Cubane*, at Ruhr Universitat, Bochum, Germany (Host: Prof. H. Zabel) July 1997.

84. *Theory of Inelastic Neutron Scattering*, at the NCNR Workshop on Cold Neutron Spectroscopy, NIST, Gaithersburg, MD, August 1997.

85. *Ordering due to Disorder in Frustrated Quantum Magnetic Systems*, at the "4th Statistical Physics Meeting", Istanbul, Turkey July 1997.

86. *First Principles Approach to Intermolecular Interactions in Solid C_{60}*, at the University of Antwerpen, Belgium (Host: Prof. K.H. Michel) July 1997.

87. *First Principles Study of Structure and Dynamics of Solid Cubane*, at the European Materials Research Society Meeting, Strasbourg, France, June 1997.

88. *Synthesis and Properties of Mixed Alkali-Alkaline Earth Fullerides*, at the Institut Charles Sadron, Strasbourg, France, June 1997.

89. *Variable Valence and Superconductivity in Fullerides*, at the American Physical Society meeting Kansas City, MO, March 1997.

90. *T_c vs. carrier concentration in cubic fulleride superconductors*, at the 189th Electrochemical Society Meeting, Los Angeles, CA, May 1996.

91. *Superconductivity in doped-fullerenes*, at Ohio University, Athens, OH (Host: Prof. R.L. Cappelletti) April 1996.

92. *T_c vs. carrier concentration in cubic fulleride superconductors*, at the Workshop on New Perspectives in Unconventional Superconducting Materials, Pisa, Italy, January 1996.

93. *Three-dimensional Ordering in bct Antiferromagnets due to Quantum Disorder*, at the University of Pennsylvania, Philadelphia, PA (Host: Prof. A.B. Harris) April 1995.

94. *Structure and Dynamics of Na_xC_{60}*, at Argonne National Laboratory, Argonne, Illinois (Host: Dr. J.D. Jorgensen) May 1994.

95. *Intermolecular Potentials and Theory for the Observation of Librons in Solid C_{60}*, at the International Winterschool on Electronic Properties of Novel Materials, Kirchberg, Austria, March 1994.

96. *Orientational Ordering of C_{60} in Na-Doped Systems*, at the American Physical Society Meeting, Pittsburgh, PA, March 1994.

97. *Orientational Order/Disorder in Na_xC_{60}*, at the International Winterschool on Electronic Properties of Novel Materials, Kirchberg, Austria, March 1994.

98. *Neutron and X-ray Study of Na-doped C_{60} compounds* at the NIST Center for Neutron Research Gaithersburg, MD (Host: Dr. D.A. Neumann) March, 1994.

99. *Phase Diagram of Na-doped C_{60}*, at the IBM Thomas J. Watson Research Center, Yorktown Heights, NY (Host: Dr. D.P. DiVincenzo) February 1994.

100. *Anisotropic Spin Hamiltonian due to Spin-Orbit and Coulomb Exchange Interactions and Spin Structure of Tetragonal Lamellar Copper Oxides*, at the IBM Thomas J. Watson Research Center, Yorktown Heights, NY (Host: Dr. D.P. DiVincenzo) February 1994.

101. *Spin Structure of Tetragonal Lamellar Copper Oxides*, at the NEC Research Institute, Princeton, NJ (Host: Dr. N. Wingreen) February 1994.

102. *Orientational Phase Transition in Na_xC_{60}*, at AT&T Bell Laboratories, Murray Hill, NJ (Host: Dr. A.P. Ramirez) February 1994.

103. *Na-doped C_{60} compounds*, at Brookhaven National Laboratory, Upton, NY (Host: Dr. J.D. Axe) February 1994.

104. *Intercalation of sodium heterocluster into the C_{60} lattice*, at the Materials Research Society Meeting, Boston, MA, November 1993.

105. *Theory of Orientational Phase Transition in C_{60}*, at the University of Montpellier, Montpellier, France (Host: Prof. P. Bernier) June 1993.