Leonardo Pisani

PERSONAL DETAILS

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POSTDOCTORAL EXPERIENCE

Nov. 2005 - Nov. 2007 Imperial College London, Chemistry Dept.:
In collaboration with Prof. N. M. Harrison (Imperial College London and CCLRC) and Dr. Barbara Montanari (CCLR Rutherford Appleton Laboratory).
The current generation of very large scale integration semiconductor devices have almost reached the quantum limits of performance with gate lengths approaching 5nm. A semiconductor, ferromagnetic at room temperature, with a highly tunable band gap and magnetic coupling could cause a revolution in nanoelectronics, providing the basis for devices which exploit the electronic spin on a sub 1nm length scale. In this project we predict that a graphene sheet with metal-free defects is a ferromagnetic semiconductor at room temperature, by using first principles calculations. Our work discovers that these purely sp-bonded systems can display room temperature ferromagnetism, a fact that challenges the foundations of the theory of magnetism. Moreover, we show that the control of defect concentration would lead to tunable band gap and magnetic coupling, opening the possibility of highly controllable graphene-based spintronics nanodevices.
Prior to this work, we performed Density Functional Theory studies on the model systems of graphitic ribbons where we demonstrated that ribbons with zig-zag edges are unstable with respect to magnetic polarisation of the edge states and that the magnetic interaction between those edge states is remarkably long ranged.
This project is part of a european collaboration between research groups in United Kingdom, Italy, Spain, Germany, Sweden and Russia (Ferrocarbon Consortium, http://www.ferrocarbon.it/).

2003-2005 J.W. Goethe Universitaet, Frankfurt am Main, Institut fuer Theoretische Physik:
In collaboration with Prof. R. Valenti two projects were developed within the approach of Density Functional Theory: 1) the study of the electronic and magnetic properties of transition-metal oxides and 2) possible spintronics applications of magnetically doped spinel semiconductors. 1) The structural and vibrational properties of the low dimensional spin 1/2 material TiOCl were investigated by a comparison between standard exchange-correlation functionals (LDA, GGA, LDA+U). The inclusion of orbital dependent correlation (as implemented in the LDA+U scheme) has proven to be essential for a correct description of these

compound. In collaboration with Prof. R. Claessen we compared our band structure calculations with angle resolved photoemission spectra revealing non-single particle effects which are still being investigated. 2) The iron substituted spinel ZnGa2O4 was investigated as a function of doping concentration and of the position of the dopant (tetrahedral and/or octahedral site). The transport and magnetic properties were studied and possible strategies for its application in spintronics were oulined.

Feb.-July '03 University of Camerino (Italy):
In collaboration with Prof. G. C. Strinati, Dr. P. Pieri and Dr. A. Perali the Bardeen-Cooper-Schreiffer–Bose-Einstein Condensation crossover for a system of trapped Fermi atoms at finite temperature, both below and above the superfluid critical temperature, was studied by including Cooper pairing fluctuations beyond mean field. Density profiles in the trap as a function of temperature and coupling strength were obtained and shown to be in good agreement with the experimental density profile of a gas of Li atoms. Predictions for the chemical potential and the excitation gap were compared with zero-temperature Quantum Monte Carlo results and found to have a remarkably good agreement.

EDUCATION

'00-Jan. '03 University of Camerino (Italy): PhD under the supervision of Prof. G. C. Strinati and Dr. P. Pieri. The work focused on the effects of Cooper pairing fluctuations on the single-particle spectra for the superconducting state of the high temperature superconductors. Several features of the single-particle spectral function were shown to compare favourably with experimental data for cuprate superconductors.

1999 Military Service

1998 University of Bologna (Italy): Undergraduate thesis under the supervision of Prof. G. Morandi. The topic of my thesis was the phase diagram of the Hubbard model in the strong coupling limit. I graduated with marks 110/110 cum laude.

1992-1997 University of Bologna (Italy): Corso di Laurea in Fisica. My studied were directed towards fundamentals of theoretical physics (quantum electrodynamics, statistical mechanics, special and general theory of relativity, classical and quantum field theory, hamiltonian dynamical systems).

1987-1992 Liceo Scientifico, Macerata, MC, (Italy): Diploma di Maturità Scientifica.

CURRENT SCIENTIFIC PROJECTS

- In collaboration with Dr. B. Montanari (Rutherford Appleton Lab.) and Prof. N.M. Harrison (Imperial College/Rutherford Appleton Lab.), *first-principles* study of magnetism in defective graphitic systems.
- In collaboration with Prof. N.M. Harrison, Dr. B. Montanari, Dr. S. Bennington, Dr. C Williams (Imperial College London) and Miss G. De Fusco

(PhD student at Imperial College), room temperature ferromagnetism in organic and metallorganic materials.

- In collaboration with Prof. R. Valenti (J.W. Goethe Universitaet, Frankfurt am Main), study of the anomalous Spin-Peierls transition and pressure induced insulator-to-metal transition in the low-dimensional quantum magnet TiOCl.
- In collaboration with Herr M. Lauer (Universitaet des Saarlandes) and Prof. R. Valenti, *first principles* study of the structural properties of the spinel FeGa2O4.
- In collaboration with Prof. M. Vozmediano (University Carlos III de, Madrid), role of topological defects in the conductivity of graphene.

SCIENTIFIC RESEARCH EXPERTISE AND INTERESTS

- Experience in *first principles* calculations based on Density Functional Theory (DFT). Applications include electronic, structural, magnetic and vibrational properties of transition metal oxides, spinel semiconductors, only-carbon systems, organic and metallorganic polymers.
- Expert user of *first principles* codes: CRYSTAL (Daresbury-Turin), WIEN2k (Vienna), CASTEP (Cambridge), and the empirical package GULP (Imperial College London).
- Experience in *quantum many-body theory*: Green's functions and diagrammatic many-body theory, Bethe-Salpeter equation and T-matrix approximation, path integrals, theory of superconductivity and superfluidity, low and high temperature superconductor materials, Bogoliubov theory of weakly interacting Bose gas, theory of the BCS-BEC crossover, condensation of bosonic and fermionic atomic gases.
- Fortran 77 and 90 programming for the computation of quantum many-body properties.

TEACHING AND SUPERVISING EXPERIENCE

- supervision of the PhD student Giulia de Fusco at Imperial College (2006-2009) in the project:”Room temperature feromagnetism in organic and metallorganic materials”
- supervision of 3rd year undergraduate student Gabriel Kan for the Literature BSc projects on Intercalated graphite (March-June 2007).
- supervision of 3rd year undergraduate student Gabriel Kan for the Literature BSc projects on Spintronics (January-March 2007).
- MRes and 4th year studentsAutumn Term 2006- Chemistry- Lecture on Magnetism and Spin-Density Functional Theory.
- 2nd year Undergraduate Autumn Term 2006- Chemistry – Problem Class -Theoretical methods in chemistry: LCAO Theory of Ethene and Butadiene.
- 2nd year Undergraduate, Spring Term 2005- Chemistry - Computational Laboratory - Module: ''The Free Energy and Thermal Expansion of MgO''
- 2nd year Undergraduate Spring Term 2005- Chemistry – Problem Class -Theoretical methods in chemistry: sequences, series, Morse potential, harmonic approximation, vibrational modes.

- Problems in quantum mechanics at the Institute for Theoretical Physics, Frankfurt am Main (3rd year Undergraduate, Winter Term 2004)

GRANT PROPOSALS

- *"Defect induced magnetism in transition metal-free compounds"*, to be submitted to EPSRC.
- *"Room temperature ferromagentism in organic and metallorganic materials",* Centre for Materials Physics and Chemistry grant, funded. I am principal investigator of the Imperial College node. The grant funds a 3-year PhD position held by Miss G. de Fusco started on November 2006.
- *"Combined optical and magnetic response of a polymer semiconductor*", proposal accepted for BSc and MSc projects (2006/2007) Chemistry Dept., Imperial College.
- *"Statistical physics of classical and quantum complex systems",* six-month grant to work on the topic of condensed atomic gases in collaboration with Prof. G.C Strinati, Dr. P. Pieri and Dr. A . Perali (2003).

CONFERENCES and WORKSHOPS

- *"Condensed Matter and Materials Physics (CMMP07)",* 12 - 13 April 2007 University of Leicester, UK. Poster:"Ferromagnetism in graphitic ribbons"
- *"Korrelationstage 2007",* 26 Feb.-2 March 2007, Max-Planck-Institut fuer Physik komplexer Systeme, Dresden, Germany. Oral contribution:"Ab-initio phonons in the Spin-Peierls phase of TiOCl"
- Annual IoP Condensed Matter Theory group meeting, University of Warwick, 19 December 2006. Poster:"Ferromagnetism in graphitic ribbons"
- *"Computational Magnetism",* 13 December 2006, The Institute of Physics, London.
- ''*CRIM06: Current research in magnetism 2006*'', 8 December 2006, London, Imperial College London.
- *"Theoretical and Experimental Magnetism Meeting*", 3-4 August 2006, Cosener's House, Abingdon, UK. Poster contribution: "Ferromagnetism in only-carbon structures".
- *"14th European Conference on Mathematics for Industry*" ,10-14 July 2006, Madrid. Oral contribution:" *Ferromagnetism in graphitic systems*".
- ''*Topics in Nano-Magnetism*'', 30 November 2005, Daresbury, UK organised by Prof W. Temmerman, Dr W. Hofer, Dr A. Wander and Prof N. Harrison.
- *"Toward atomistic materials design",* Ψk Conference, 17-21 September, 2005, Schwaebisch Gmuend, Germany. Poster Contribution: "Ab-initio phonons for the layered compound TiOCl".
- Spring Meeting of the Condensed Matter Division of the German Physical Society, DPG, Berlin (4-9 March, 2005). Poster Contribution: "Ab-initio phonons for the layered compound TiOCl".

- International workshop on "*Collective quantum states in low-dimensional transition metal oxides*", 22-25 Feb.2005, Max Planck Insitut fuer Physik Komplexer, Dresden (Germany).
- "*Field Theory of Quantum Coherence, Correlations, and Mesoscopics*'', III Windsor Summer School, Windsor (Lancaster University, UK), 9-22 August 2004. Poster contribution: "BCS-BEC crossover at finite temperature for superfluid trapped Fermi atoms".
- XI National School of the Physics of Condensed Matter "*Stati elettronici in metalli superconduttori*" Sep. 2000, I.S.I. Foundation (Institute for Scientific Interchange), Villa Gualino, (Turin, Italy).

MEMBERSHIP OF PROFESSIONAL SOCIETIES and REFERRED JOURNALS

- Member of The American Physical Society
- Corporate Member of The Institute of Physics
- Referee of Physical Review B
- Referee of Journal of Physics: Condensed Matter
- Referee of Journal of Physics: Applied Physics

PUBLICATIONS

Articles:

17. G. C. de Fusco, L. Pisani, B. Montanari, N. H. Harrison, *"Electronic and magnetic properties of $V(TCNE)_2$"*, in preparation.
16. L. Pisani, B. Montanari, N. H. Harrison, *"Invalidation of a putative ferromagnetic structure of carbon"*, in preparation.
15. L. Pisani, R. Valenti, B. Montanari and N. M. Harrison, "*Density functional study of the electronic and vibrational properties of TiOCl*", Phys. Rev. B. **76**, 235126 (2007)
14. L. Pisani, B. Montanari, N. H. Harrison, *"Defective Graphene-A ferromagnetic Semicondutor"*, submitted to New Journal of Physics.
13. L. Pisani, J. A. Chan, B. Montanari, N. H. Harrison,"*Electronic and Magnetic Structure of graphitic ribbons*", Phys. Rev. B. **75**, 064418 (2007)
12. M. Hoinkis, M. Sing, S. Glawion, L. Pisani, R. Valenti, S. van Smaalen, M. Klemm, S. Horn, and R. Claessen**, "***One-dimensional versus two-dimensional correlation effects in the oxyhalides TiOCl and TiOBr***",** Phys. Rev. B **75**, 245124 (2007)
11. L. Pisani, T. Maitra, and R. Valenti:"*Effects of Fe substitution on the electronic, transport, and magnetic properties of ZnGa2O4: A systematic ab initio study*", Phys. Rev. B, **73,** 205204 (2006)
10. M. Sing, M. Hoinkis, J. Schaefer, M. Klemm, S. Horn, H. Benthien, E. Jeckelmann, L. Pisani, R. Valenti, and R. Claessen*:"Electronic structure and fluctuation effects in the spin-1/2 quantum magnet TiOCl",* J. de Physique IV **131,** 331 (2005)
9. M. Hoinkis, M. Sing, J. Schaefer, M. Klemm, S. Horn, H. Benthien, E. Jeckelmann, T.Saha Dasgupta, L. Pisani, R. Valenti, and R. Claessen: "*Electronic structure of the spin-1/2 quantum magnet TiOCl*", Phys. Rev. B, **72,** 125127 (2005)

8. L. Pisani and R. Valenti: “ *Ab initio phonon calculations for the layered compound TiOCl”,* Phys. Rev. B, **71** , 180409(R) (2004)
7. P. Pieri, L. Pisani, and G. C. Strinati:”*Comparison between a diagrammatic theory for the BCS-BEC crossover and quantum Monte Carlo results*”, Phys. Rev. B, **73,** 0125127 (2005)
6. A. Perali, P. Pieri, L. Pisani, and G. C. Strinati:”*BCS-BEC Crossover at Finite Temperature for Superfluid Trapped Fermi Atoms”,* Phys. Rev. Lett., **92,** 220404 (2004)
5. P. Pieri, L. Pisani, G. C. Strinati and A. Perali*:”Single-particle spectra and magnetic field effects within precursor superconductivity”,* PHYSICA C **408,** 317 (2004)
4. P. Pieri, L. Pisani, and G. C. Strinati:”*Pairing Fluctuation Effects on the Single-Particle Spectra for the Superconducting State”,* Phys. Rev. Lett., **92,** 110401 (2004)
3. P. Pieri, L. Pisani, and G. C. Strinati: ”*BCS-BEC crossover at finite temperature in the broken-symmetry phase”*, Phys. Rev. B, **70**, 094508 (2004)
2. E. Ercolessi., G. Morandi, L. Pisani and M. Roncaglia:”*Mixed phases for the t-J model*”, Physica C **331,** 178 (2000)
1. L. Pisani: “*Magnetic properties in strongly correlated electron system*'' Degree Thesis, Faculty of Science, University of Bologna, Oct. 1998