

SEMS: Spectroscopies, Electron correlations, Modeling-Simulations and low-dimensional systems

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Research Activity

Our theoretical study in collaboration focused on:

- Electron spectroscopy of magnetic systems,
- The fundamental properties of carbon nanotubes and graphene interconnects
- Energy functional of ensemble density functional theory (DFT) in systems with attractive interactions
- Scissors modes in crystals.
- Multiple scattering expansions.

Awards in the Year 2015

2015 IMS (International Microwave Symposium) Student Design Competition Winner: presented as part of the student design competitions at the 2015 IEEE Microwave Theory and Techniques Society (MTT -S) International Microwave Symposium. Awarded for the app described in the article: M. Baldelli, L. Pierantoni, S. Bellucci, Learning by Using Graphene Multilayers, IEEE Microwave Magazine (Volume: 17, Issue: 1), pp. 44 – 51, Date of publication: 10 December 2015

List of Conference Talks in the Year 2015

S. Bellucci, Graphene materials for electronic and electromagnetic applications, 27th Indian-Summer School on Graphene - the Bridge between Low- and High-Energy Physics, September 14 - 18, 2015, Prague, Czech Republic.

S. Bellucci, Electromagnetic characterization of graphene and graphene nanoribbons via ab-initio permittivity simulations, Is quantum theory exact? The endeavor for the theory beyond standard quantum mechanics. Second Edition FQT2015, INFN-LNF, Frascati (Italy), Sept. 23-25, 2015

S. Bellucci, Ballistic Ratchet effect on patterned graphene, FM&NT-2015 | Functional Materials and Nanotechnologies, Vilnius (Lithuania), 5-8 October 2015

S. Bellucci, Electrical conductivity of graphene: a time-dependent density functional theory study, Semiconductor Conference (CAS), 2015 International, Sinaia (Romania) 13 - 15 October 2015.

S. Bellucci, Excitation of surface waves at terahertz frequencies on a suspended graphene sheet, 2nd Bilateral Indo - Italian Workshop October 11-14, 2015 NEEM2015 CNR Roma (Italy).

S. Bellucci, What Next in Condensed Matter, INFN-LNF, Frascati (Italy), Feb 27, 2015.

S. Bellucci, Research Seminar, Unical Cosenza (Italy), 10 March 2015

S. Bellucci, Broadband electromagnetic response and applications of graphene related materials, NATO Advanced Research Workshop on Fundamental and Applied NanoElectroMagnetics, FANEM 2015, Minsk, Belarus, May 25-27 2015

S. Bellucci, Electromagnetic characterization of graphene and Graphene nanoribbons via ab-initio permittivity simulations, International Conference on Electromagnetics in Advanced Applications (ICEAA 2015), Turin (Italy), Sept. 7-11, 2015

A. Maffucci, Synthesis and electrical characterization of graphene nanoplatelets, Electromagnetic characterization of graphene and Graphene nanoribbons via ab-initio permittivity simulations, International Conference on Electromagnetics in Advanced Applications (ICEAA 2015), Turin (Italy), Sept. 7-11, 2015

A. Maffucci, Circuitual Representation of Quantum Devices in Entangled States, Nanoscience and Nanotechnology 2015, INFN-LNF Frascati (Italy), 28 September - 02 October 2015.

F. Micciulla, Novel bottom -up process to realize graphene based devices, Nanoscience and Nanotechnology 2015, INFN-LNF Frascati (Italy), 28 September - 02 October 2015.

D. Mencarelli, Analysis and characterization of nanoscale devices based on new low dimensional materials, Nanoscience and Nanotechnology 2015, INFN-LNF Frascati (Italy), 28 September - 02 October 2015.

G. Stefanucci, New diagrammatic expansion for approximations with positive spectral properties, Nanoscience and Nanotechnology 2015, INFN-LNF Frascati (Italy), 28 September - 02 October 2015.

L. Pierantoni, Time-domain multiphysics modeling of the electromagnetic-transport problem in nanomaterials/devices: a new challenge in computational engineering, Nanoscience and Nanotechnology 2015, INFN-LNF Frascati (Italy), 28 September - 02 October 2015.

A. Tagliacozzo, Probing deep interface electron-phonon interaction in Bi₂Te₃/ Ga As with Brillouin

scattering: experiment and DFT modeling of the interface with the topological insulator, Nanoscience and Nanotechnology 2015, INFN-LNF Frascati (Italy), 28 September - 02 October 2015.

Publications by LNF Authors in the Year 2015

G Stefanucci, S Kurth, Steady-State Density Functional Theory for Finite Bias Conductances
Nano letters 15 (12), 8020-8025 (2015)

E Perfetto, D Sangalli, A Marini, G Stefanucci, Nonequilibrium Bethe-Salpeter equation for transient photoabsorption spectroscopy, Physical Review B 92 (20), 205304 (2015)

E Perfetto, AM Uimonen, R van Leeuwen, G Stefanucci, First-principles nonequilibrium Green's-function approach to transient photoabsorption: Application to atoms, Physical Review A 92 (3), 033419 (2015)

E Perfetto, G Stefanucci, Some exact properties of the nonequilibrium response function for transient photoabsorption, Physical Review A 91 (3), 033416 (2015)

AM Uimonen, G Stefanucci, Y Pavlyukh, R van Leeuwen, Diagrammatic expansion for positive density-response spectra: Application to the electron gas, Physical Review B 91 (11), 115104 (2015)

E Perfetto, G Stefanucci, Transient dynamics in the Anderson–Holstein model with interfacial screening, Journal of Computational Electronics 14 (1), 352-359 (2015)

P Frank, M Benfatto, M Qayyam, B Hedman, KO Hodgson A high-resolution XAS study of aqueous Cu(II) in liquid and frozen solutions: Pyramidal, polymorphic, and non-centrosymmetric, J. Chem. Phys. 142, 084310 (2015)

M Benfatto, C Meneghini, A close look into the low energy region of the XAS spectra: the XANES region, Synchrotron Radiation, Springer, pp. 213-240, 2015

J Xu, P Krüger, CR Natoli, K Hayakawa, Z Wu, K Hatada, X-ray absorption spectra of graphene and graphene oxide by full-potential multiple scattering calculations with self-consistent charge density, Physical Review B 92 (12), 125408 (2015)

J Bartolomé, F Bartolomé, AI Figueroa, O Bunău, IK Schuller, T Gredig, F Wilhelm, A Rogalev, P Krüger, CR Natoli, Quadrupolar XMCD at the Fe K-edge in Fe phthalocyanine film on Au: Insight into the magnetic ground state, Physical Review B 91 (22), 220401 (2015)

F Bartolomé, O Bunău, LM García, CR Natoli, M Piantek, JI Pascual, IK Schuller, T Gredig, F Wilhelm, A Rogalev, J Bartolomé, Molecular tilting and columnar stacking of Fe phthalocyanine thin films on Au (111), Journal of Applied Physics 117 (17), 17A735 (2015)

F Palumbo, Composites and quasiparticles in a number conserving bosonization method
Journal of Superconductivity and Novel Magnetism, 1-3 (2015)

Collapse and hybridization of RNA: view from replica technique approach, Y. Sh. Mamasakhlisov, S. Bellucci, Sh. Hayryan, H. Caturyan, Z. Grigoryan, and C.-K. Hu, The European Physical Journal E 38, 1-9 (2015)

What does See the Impulse Acoustic Microscopy inside Nanocomposites?

VM Levin, YS Petronyuk, ES Morokov, A Celzard, S Bellucci, PP Kuzhir, Physics Procedia 70, 703-706 (2015).

Electromagnetic characterization of graphene and graphene nanoribbons via ab-initio permittivity simulations, S Bellucci, A Sindona, D Mencarelli, L Pierantoni, 2015 International Conference on Electromagnetics in Advanced Applications (ICEAA), 926-929, Editor IEEE.

Synthesis and electrical characterization of Graphene Nanoplatelets, A Maffucci, F Micciulla, A Cataldo, G Miano, S Bellucci, 2015 International Conference on Electromagnetics in Advanced Applications (ICEAA), 301-304, Editor IEEE.

Applications of Graphene at Microwave Frequencies, M. Bozzi, L Pierantoni, S Bellucci, Radioengineering 24 (3), 661 (2015).

Broadband Microwave Attenuator Based on Few Layer Graphene Flakes, L Pierantoni, D Mencarelli, M Bozzi, R Moro, S Moscato, L Perregrini, F. Micciulla, A. Cataldo, S. Bellucci, IEEE Transactions on Microwave Theory and Techniques, Aug. 2015, vol. 63, no. 8, p. 2491–2497. DOI: 10.1109/TMTT.2015.2441062.

Spatial dispersion effects upon local excitation of extrinsic plasmons in a graphene micro-disk, D Mencarelli, S Bellucci, A Sindona, L Pierantoni, arXiv preprint arXiv:1507.07090661 Journal of Physics D: Applied Physics (2015).

On the absence of actual plateaus in zero-temperature magnetization curves of quantum spin clusters and chains, V Ohanyan, O Rojas, J Strecka, S Bellucci, Physical Review B 92 (21), 214423, arXiv preprint arXiv:1506.02933 (2015).

Volume reflection and volume capture of ultrarelativistic particles in bent single crystals

S Bellucci, YA Chesnokov, VA Maishev, IA Yazynin

Physical Review Special Topics-Accelerators and Beams 18 (11), 114701 (2015)

Design, fabrication and electrical characterization of a low-cost and solvent-free graphene electronic device, A Maffucci, F Micciulla, A Cataldo, G Miano, S Bellucci, IEEE International Conference on Microwaves, Communications, Antennas and Electronic Systems (COMCAS), pp. 1-4, 2015

Electrical conductivity of graphene: a time-dependent density functional theory study

S Bellucci, A Sindona, D Mencarelli, L Pierantoni, 2015 International Semiconductor Conference (CAS), 203-206 (2015).

Electromagnetic characterization of graphene and graphene nanoribbons via ab-initio permittivity simulations, S Bellucci, A Sindona, D Mencarelli, L Pierantoni, 2015 International Conference on Electromagnetics in Advanced Applications (ICEAA), pp. 926-929, (2015)

Synthesis and electrical characterization of Graphene Nanoplatelets, A Maffucci, F Micciulla, A Cataldo, G Miano, S Bellucci, 2015 International Conference on Electromagnetics in Advanced Applications (ICEAA), pp. 301-304, (2015)

Broadband Dielectric Spectroscopy of Composites Filled With Various Carbon Materials, S Bellucci, S Bistarelli, A Cataldo, F Micciulla, I Kranauskaite, ..., Microwave Theory and Techniques, IEEE Transactions on 63 (6), 2024-2031 (2015)

Comparison of rigorous vs approximate methods for accurate calculation of 2D-materials band structures and applications to THz nanoelectronics, L Pierantoni, D Mencarelli, A Sindona, S Bellucci Microwave Symposium (IMS), 2015 IEEE MTT-S International, 1-3

Innovative full wave modeling of plasmon propagation in graphene by dielectric permittivity simulations based on density functional theory

L Pierantoni, D Mencarelli, A Sindona, M Gravina, M Pisarra, CV Gomez, S Bellucci, Microwave Symposium (IMS), 2015 IEEE MTT-S International, 1-3

Electromagnetic properties of graphene nanoplatelets/epoxy composites in the wide temperature range A Plyushch, J Macutkevicius, J Banys, D Bychanok, S Maksimenko, A Cataldo, F Micciulla, S Bellucci, Proceedings of International Conference Nanomeeting–2015 Physics, Chemistry and Applications of Nanostructures pp. 233-235 (2015)

Thermodynamic curvature for a two-parameter spin model with frustration

G Ruppeiner, S Bellucci, Physical Review E 91 (1), 012116 (2015)

CNTs-and GNRs-based electromagnetic and spintronic devices: models and simulations

YN Shunin, YF Zhukovskii, VI Gopeyenko, NY Burlutskaya, TD Lobanova-Shunina, S Bellucci, Proceedings of International Conference Nanomeeting–2015 Physics, Chemistry and Applications of Nanostructures pp. 207-210 (2015)

Microstructure, elastic and electromagnetic properties of epoxy-graphite composites, S Bellucci, F Micciulla, VM Levin, YS Petroniyuk, LA Chernozatonskii, PP Kuzhir, AG Paddubskaya, J Macutkevicius, MA Pletnev, V Fierro, A Celzard, AIP Advances 5 (6), 067137 (2015).

Multiwalled carbon nanotube buckypaper induces cell cycle arrest and apoptosis in human leukemia cell lines through modulation of AKT and MAPK signaling pathways, S Dinicola, MG Masiello, S Proietti, P Coluccia, G Fabrizi, A Palombo, F. Micciulla, S. Bistarelli, G. Ricci, A. Catizone, G. De Toma, M. Bizzarri, S. Bellucci, A. Cucina, Toxicology in Vitro 29, 1298–1308 (2015).

Growth inhibition, cell-cycle alteration and apoptosis in stimulated human peripheral blood lymphocytes by multiwalled carbon nanotube buckypaper, O Zeni, A Sannino, S Romeo, F Micciulla, S Bellucci, MR Scarfi, Nanomedicine 10 (3), 351-360 (2015).

Sharp variations in the electronic properties of graphene deposited on the h-BN layer, DG Kvashnin, S Bellucci, LA Chernozatonskii, Physical Chemistry Chemical Physics 17 (6), 4354-4359 (2015).

Biological interactions of carbon-based nanomaterials: From coronation to degradation, K Bhattacharya, SP Mukherjee, A Gallud, SC Burkert, S Bistarelli, S. Bellucci, M. Bottini, A. Star, B. Fadeel, Nanomedicine: Nanotechnology, Biology and Medicine, Volume 12, Issue 2, February 2016, Pages 333–351

YN Shunin, S Bellucci, YF Zhukovskii, VI Gopeyenko, NY Burlutskaya, TD Lobanova-Shunina, Nanocarbon electromagnetics in CNT-, GNR-and aerogel-based nanodevices: models and simulations, Computer Modelling & New Technologies 2015 19 (1A) 35-42

M. Baldelli, L. Pierantoni, S. Bellucci, Learning by Using Graphene Multilayers, IEEE Microwave Magazine (Volume:17 , Issue: 1), pp. 44 – 51, Date of publication: 10 December 2015