ALLEGATO B

UNIVERSITÀ DEGLI STUDI DI MILANO
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Marco Cazzaniga
CURRICULUM VITAE

INFORMAZIONI PERSONALI (NON INSERIRE INDIRIZZO PRIVATO E TELEFONO FISSO O CELLULARE)

COGNOME	CAZZANIGA
NOME	MARCO
DATA DI NASCITA	28/10/1981

EDUCATION

December 22, 2008 - PhD in Physics, Astrophysics, and Applied Physics at the Università degli Studi di Milano. Thesis title: *Ab-initio approach to density-response and excitation spectra in metallic systems.* Supervisor Prof. Giovanni Onida. Stage at the LSI at the Ecole Polytechnique in the period April-July 2007 (Palaiseau F).

July 14, 2005 – Laurea magistrale in Physics at the Università degli Studi di Milano, with 110/110 cum laude. Curriculum of condensed matter physics. Thesis title: *Computation of electronic properties of metallic surfaces: total energy and quasiparticle excitations*. Supervisor prof. Giovanni Onida.

RESEARCH EXPERIENCES

March 1, 2019 – Present – Collaboration contract ("Co. Co. Co.") at the Università degli studi di Milano to perform research activity on vibrational spectroscopy of adsorbates on TiO_2. Group of Prof. Michele Ceotto.

September 1, 2017 – Septembre 22, 2018 (suspended for 22 days in June/July 2018) – PostDoc ("Assegno di ricerca - art. 22 della Legge n. 240/2010") at the Università degli studi di Milano to perform research activity on vibrational spectroscopy of adsorbates on TiO_2. Group of Prof. Michele Ceotto.

February 2, 2015 – August 1, 2017 - PostDoc ("Assegno di ricerca - art. 22 della Legge n. 240/2010") at the ISTM-CNR to perform research activity on chemical degradation of molecules for OLED devices and exciplex formation. Group of Dr. Davide Ceresoli

November 1, 2011 – November 14, 2013 (suspended for 14 days in october 2012) – PostDoc ("Assegno di ricerca - art. 22 della Legge n. 240/2010") at the Università degli studi di Milano to perform research activity in collaboration with STMicroelectronics (Central CAD and Design Solution department) on investigation on substrate crosstalk effects in System on Chip for automotive applications. Group of Prof. Valentino Liberali.

May 12, 2011 – June 11, 2011 – Collaboration contract ("Co. Co. Co.") at the Università degli studi di Milano to investigate electronic properties of a-Si:H/c-Si interfaces. Group of Prof. Giovanni Onida.

January 1, 2009 – December 31, 2010 – PostDoc ("Assegno di ricerca - art. 51, comma 6 della Legge n. 449/1997") at the Università degli studi di Milano to perform research activity on excited state properties in condensed matter systems within the European Theoretical Spectroscopy Facility (ETSF). Group of Prof. Giovanni Onida.

RESEARCH INTERESTS

Research interests and current projects

1. Ab initio calculation of excited state properties of condensed matter (Time-Dependent Density-Functional Theory and GW Approximation).
2. Ab initio Car-Parrinello and Born-Oppenheimer molecular dynamic.
3. Semiclassical Dynamics.
4. Calculation of vibrational properties of molecules adsorbed on oxide surfaces.

Past projects

1. Investigation of the mechanisms of formation of exciplexes between organic molecules.
2. Calculation of absorption and emission spectra in organic molecules for application in OLEDs.
3. Ab initio simulations of dielectric properties of solids (optical response, electron energy loss, and inelastic X-ray scattering spectra) thanks to TD-DFT
4. Investigation on the origin of the Charge Density Wave instability in $TiSe_2$.
5. Calculation of quasiparticle properties of metals (energies, lifetimes and spectral functions) through the GW approximation.
6. Study of electronic properties of interfaces for photovoltaic applications.
7. TD-DFT simulations of electron energy loss in MAX phases.
8. Contribution to the development of the TD-DFT linear response implementation of the dp-code.
9. Analysis of substrate crosstalk effects in System on Chip for automotive applications.

LANGUAGES

Italian: mother tongue; English: good proficiency, both written and oral.

PUBLICATIONS

Author of 20 publications (16 in peer-reviewed journals and 4 conference proceedings)
H-index: 8 (source: Web of Science)

A- Papers in peer-reviewed journals

1. *Unraveling the Degradation Mechanism of FIrpic-Based Blue OLEDs: I. A Theoretical Investigation*, Marco Cazzaniga, Fausto Cargnoni, Marta Penconi, Alberto Bossi, and Davide Ceresoli, Chem. Mater. **31**, 2269 (2019); 1 citations
2. *Unraveling the Degradation Mechanism in FIrpic-Based Blue OLEDs: II. Trap and Detect Molecules at the Interfaces*, Marta Penconi, Marco Cazzaniga, Walter Panzeri, Andrea Mele, Fausto Cargnoni, Davide Ceresoli, and Alberto Bossi, Chem. Mater. **31**, 2277 (2019); 1 citations
3. *β-Diketonate ancillary ligands in heteroleptic iridium complexes: a balance between synthetic advantages and photophysical troubles*, Marta Penconi, Marco Cazzaniga, Sagar Kesarkar, Clara Baldoli, Patrizia R. Mussini, Davide Ceresoli, and Alberto Bossi, *Photochem. Photobiol. Sci. 17, 1169 (2018)*; 1 citations
4. *π–π-Induced aggregation and single-crystal fluorescence anisotropy of 5,6,10b-triazaacephenanthrylene*, Katarzyna Ostrowska, Davide Ceresoli, Katarzyna Stadnicka, Marlena Gryl, Marco Cazzaniga, Raffaella Soave, Bogdan Musielak, Łukasz J. Witek, Piotr Goszczycki, Jarosław Grolik and Andrzej M. Turek, IUCrJ **5**, 335 (2018); 2 citations.
5. *Upper limit to the ultimate achievable emission wavelength in near-IR emitting cyclometalated Iridium complexes*, Marta Penconi, Marco Cazzaniga, Sagar Kesarkar, Patrizia R. Mussini, Davide Ceresoli, and Alberto Bossi, Photochem. Photobiol. Sci. **16**, 1220 (2017); 4 citations.
6. *Near-IR Emitting Ir(III) Complexes with Heteroaromatic b-Diketonate Ancillary Ligands for Efficient Solution Processed OLEDs: Structure-Property Correlations*, Sagar Kesarkar, Wojciech Mróz, Marta Penconi, Mariacecilia Pasini, Silvia Destri, Marco Cazzaniga, Davide Ceresoli, Patrizia R. Mussini, Clara Baldoli, Umberto Giovanella, and Alberto Bossi, Angewandte Chemie Int. Ed. **55**, 2714 (2016); 43 citations.
7. *Atomistic study of the structural and electronic properties of a-Si:H/c-Si interfaces*, Ivan Santos, Marco Cazzaniga, Giovanni Onida, and Luciano Colombo, J. Phys. Cond. Mat. **26**, 095001 (2014); 7 citations.
8. *Comment on "Charge-Density Wave and Superconducting Dome in $TiSe_2$ from Electron-Phonon Interaction"*, Valerio Olevano, Marco Cazzaniga, Matteo Ferri, Lucia Caramella, and Giovanni Onida, Phys. Rev. Lett. **112**, 049701 (2014); 5 citations.

9. *GW and beyond approaches to quasiparticle properties in metals*, Marco Cazzaniga, Phys. Rev. B **86**, 035120 (2012); 14 citations.
10. *Ab initio many-body effects in $TiSe_2$: A possible excitonic insulator scenario from GW band-shape renormalization*, Marco Cazzaniga, Hervé Cercellier, Markus Holzmann, Claude Monney, Philipp Aebi, Giovanni Onida, and Valerio Olevano, Phys. Rev. B **85**, 195111 (2012); 16 citations.
11. *Dynamical response function in Sodium and Aluminum from Time-Dependent Density-Functional Theory*, Marco Cazzaniga, Hans-Christian Weissker, Simo Huotari, Tuomas Pylkkänen, Paolo Salvestrini, Giulio Monaco, Giovanni Onida, and Lucia Reining, Phys. Rev. B **84**, 075109 (2011); 20 citations.
12. *Dynamical response function in sodium studied by inelastic x-ray scattering spectroscopy*, Simo Huotari, Marco Cazzaniga, Hans-Christian Weissker, Tuomas Pylkkänen, Harald Müller, Lucia Reining, Giovanni Onida, and Giulio Monaco, Phys. Rev. B **84**, 075108 (2011); 19 citations.
13. *Implementation of techniques for computing optical properties in 0-3 dimensions, including a real-space cutoff, in ABINIT*, Carlo Motta, Matteo Giantomassi, Marco Cazzaniga, Katalin Gaál-Nagy, and Xavier Gonze, Comp. Mat. Sci. **50**, 698 (2010); 11 citations.
14. *Ab initio intraband contributions to the optical properties of metals*, Marco Cazzaniga, Lucia Caramella, Nicola Manini, and Giovanni Onida, Phys. Rev. B **82**, 035104 (2010); 19 citations.
15. *Dynamic structure factor and dielectric function of silicon for finite momentum transfer: inelastic x-ray scattering experiments and ab initio calculations*, Hans-Christian Weissker, Jorge Serrano, Simo Huotari, Eleonora Luppi, Marco Cazzaniga, Fabien Bruneval, Francesco Sottile, Giulio Monaco, Valerio Olevano, and Lucia Reining, Phys. Rev. B **81**, 085104 (2010); 29 citations.
16. *Ab-initio self-energy corrections in systems with metallic screening*, Marco Cazzaniga, Nicola Manini, Luca Guido Molinari, and Giovanni Onida, Phys. Rev. B **77**, 035117 (2008); 4 citations.

B- Proceedings and other publications

1. *Evaluating the Impact of Substrate Noise on Conducted EMI in Automotive Microcontrollers*, Marco Cazzaniga, Patrice Joubert Doriol, Aurora Sanna, Emmanuel Blanc, Valentino Liberali, and Davide Pandini, Proceedings of 9th International Workshop on Electromagnetic Compatibility of Integrated Circuits (EMC Compo 2013), Nara (Japan), 15-18 December 2013, p. 129; 3 citations.
2. *Evaluating the Impact of Substrate on Power Integrity in Industrial Microcontrollers*, Marco Cazzaniga, Patrice Joubert Doriol, Emmanuel Blanc, Valentino Liberali, and Davide Pandini, Proceeding of 23rd International Workshop on Power And Timing Modeling, Optimization and Simulation (PATMOS 2013), Karlsruhe (Germany), 9-11 September 2013 , p. 107; 0 citations.
3. *Ab initio long-wavelenght properties of metallic systems: iron and magnesium*, Marco Cazzaniga, Lucia Caramella, Nicola Manini, Paolo Salvestrini, and Giovanni Onida, Epioptics-11, Proceedings of the 49th Course of the International School of Solid State Physics, Erice (Italy), 19-25 July 2010, Editor A. Cricenti, p. 30, World Scientific (2012); 0 citations.
4. *The dynamic structure factor of simple metals: a study of the electronic correlation in solids* Marco Cazzaniga, Hans-Christian Weissker, Simo Huotari, Tuomas Pylkkänen, Giulio Monaco, Lucia Reining, and Giovanni Onida, Epioptics-10, Proceedings of the 43rd Course of the International School of Solid State Physics, Erice (Italy), 21-26 June 2008, Editor A. Cricenti, p. 55, World Scientific (2010); 0 citations.

PARTICIPATION TO NATIONALLY/INTERNATIONALLY FOUNDED PROJECTS

2017 Current PostDoc at Univrsità degli Studi di Milano Under EU grant SEMICOMPLEX-ERC-2014 CoG. Principal investigator Prof. Michele Ceotto.

2015-2017 PostDoc at the ISTM-CNR founded from the Samsung-GRO project entitled: *Exciton- and polaron-induced OLED degradation by combined ab-initio molecular dynamics and experiments.* Principal Investigator Dr. Davide Ceresoli.

2009-2011 PostDoc at Univrsità degli Studi di Milano in the Milan node of the European Theoretical Spectroscopy Facility founded in the framework of the FP7 Electronic Integrated Infrastructure Initiative ('e-I3'). Node leader Prof. Giovanni Onida.

CONFERENCES AND WORKSHOPS

A- Contributions to conferences and workshops:

1. Poster *Theoretical vibrational spectroscopy of water adsorption on TiO_2 Anatase(101)* at MolSimEng (Milano, Italy, 26 September 2018)
2. Poster *Ab-initio Many Body Perturbation Theory approaches for the calculation of electronic properties of cyclometalled Ir(III) complexes* at 23rd ETSF Workshop on Electronic Excitations: Interdisciplinary Views on Quantum Many-Body Theory, (Milan 10-14 september 2018)
3. Poster *Ab-initio molecular dynamics simulations of excitation-induced OLED degradation* at 23rd ETSF Workshop on Electronic Excitations: Interdisciplinary Views on Quantum Many-Body Theory, (Milan 10-14 september 2018)
4. **Talk** *Ab-initio simulations of exciplex formation* at CECAM workshop: Multiscale modelling of organic semiconductors: from elementary processes to devices (Grenoble, France, 12-15 September 2017)
5. Poster *Ab-initio molecular dynamics simulations of excitation-induced OLED degradation* at CECAM workshop: Multiscale modelling of organic semiconductors: from elementary processes to devices (Grenoble, France, 12-15 September 2017)
6. Poster *Ab-initio molecular dynamics simulations of polaron- and exciton- induced OLED degradation* at 18 International Workshop on computational Physics and Material Science: Total energy and Force methods (ICTP-Trieste, Italy 12-14 January 2017)
7. Poster *Ab-initio molecular dynamics simulation of polaron- and exciton-OLED degradation* at CM&L conference (Bologna, Italy, 21-23 September 2015)
8. **Talk** *Ab-initio molecular dynamics simulation of polaron- and exciton-OLED degradation* at Psi-K conference (Donostia-San Sebastian, Spain, 7-10 September 2015)
9. Poster *Electron energy loss anisotropies in MAX phases: Ti_2AlC* at Psi-K conference (Donostia-San Sebastian, Spain, 7-10 September 2015)
10. **Talk** *Ab initio many-body effects in $TiSe_2$* at FISMAT 2013 (Milan, Italy, 9-13 September 2013).
11. **Invited Talk** *Ab initio many-body effects in $TiSe_2$: can GW describe an excitonic insulator?* at SPLDS 2012 (Pont-à-Mousson, France, 29 May – 1 June 2012)
12. **Talk** *Ab initio many-body effects in $TiSe_2$* at ETSF Workshop on Electronic Excitations: Bridging theory and experiment (Turin, Italy, 27-30 September 2011)
13. Poster *GW and beyond approaches to quasiparticle properties in metals* at ETSF Workshop on Electronic Excitations: Bridging theory and experiment, (Turin, Italy 27-30 September 2011)
14. Poster *GW and beyond approaches to quasiparticle properties in metals at 8 Nanoquanta Young Researchers' meeting,* (Naples, Italy 17-20 June 2011)
15. Poster *Ab initio many-body effects in $TiSe_2$ at 8 Nanoquanta Young Researchers' meeting,* (Naples, Italy 17-20 May 2011)

16. Poster *Ab initio many body effects in $TiSe_2$ at ETSF Workshop on Electronic Excitations: New Frontiers in Theoretical Spectroscopy and Quantum Transport,* (Berlin, Germany 12-15 October 2010)
17. Poster *Dynamical response function in sodium and aluminum from Time-Dependent Density Functional Theory at Psi-k conference 2010* (Berlin, Germany 12-16 September 2010)
18. **Talk** *Ab initio long-wavelength properties of metallic system: iron and magnesium* at EPIOPTICS-11 (Erice, Italy, 19-25 July 2010).
19. **Talk** *Ab-initio long wavelength dielectric properties of bulk iron* at ETSF Workshop on Electronic Excitations: Ab-initio tools for the characterization of nanostructures (Evora, Portugal, 14-19 September 2009).
20. Poster *Theoretical spectroscopies of near-free-electron metals* at 6 Nanoquanta Young Researchers' meeting, (Berlin, Germany 2-6 june 2009)
21. **Talk** *Ab-initio GW self-energy corrections in metallic systems* at the 4th ABINIT developer workshop (Autran, France, 24-27 March 2009).
22. **Talk** *The dynamic structure factor for simple metals: a study of the electronic correlation of solids* at 13 Nanoquanta-ETSF Workshop on Electronic Excitations: Theoretical spectroscopies and quantum transport (Pugnochiuso, Italy 22-27 september 2008)
23. **Talk** *The dynamic structure factor for simple metals: a study of the electronic correlation of solids* at EPIOPTICS-10 (Erice, Italy 21-26 June 2008).
24. **Talk** *The dynamic structure factor for simple metals: a study of the electronic correlation of solids* at 5th Nanoquanta Young Researchers' meeting (Modena, Italy, 20-23 May 2008).
25. Poster *Ab-initio self-energy correction in systems with metallic screening* at 12 Nanoquanta Workshop on Electronic Excitations: Time Dependent Density Functional Theory: Advances and Prospects (Aussois, France 18-22 September 2007)
26. **Talk** *Study of the small-q contribution to the polarizability and the intra-band term: from the jellium to the periodic solid* at 4th Nanoquanta Young Researchers' meeting (Donostia-San Sebastian, Spain, 15-18 May 2007).
27. Poster *Study of the small-q contribution to the polarizability and the intraband term: from the jellium to the periodic solid* at 13 International Workshop on computational Physics and Material Science: Total energy and Force methods (ICTP-Trieste, Italy 11-13 January 2007)
28. Poster *Study of the small-q contribution to the polarizability and the intraband term: from the jellium to the periodic solid* at 11 Nanoquanta Workshop on Electronic Excitations: A decade of applications of the Bethe-Salpeter Equation (Houffalize, Belgium 19-22 September 2006)
29. Poster *Evaluation of the dielectric response and quasiparticle excitations in bulk and slab jellium with an ab-initio plane-wave numerical tool* at 3 Nanoquanta Young Researchers' meeting (Rome, Italy 3-5 may 2006)

B- Participation to summer schools

1. Summer school "Quantum Monte Carlo and the Casino Program X" - Vallico di Sotto (I) – 23-30 July 2016.
2. CECAM tutorial: "Excitations in Realistic Materials using Yambo on Massively Parallel Architectures" - CECAM Lausanne (CH) 13-17 April 2015.
3. "Autumn school on numerical computing" - Caspur Roma (I) - 1-2 October 2012.
4. "Corso base di Python per la programmazione in ambito scientifico" – Cilea Segrate (I) – 22-25 March 2010.
5. Summer school "Ab initio many body theory"; Universidad del Pais Vasco S.Sebastian (E) – 22-28 July 2007.
6. CECAM tutorial: "Electronic excitations and spectroscopies: Theory and codes" – CECAM Lyon (F) - 11-15 December 2006.
7. 15° summer school on parallel computing – CINECA, Casalecchio di Reno (I) – 3-14 July 2006.

COMPUTATIONAL SKILLS

Experience in DFT, Car-Parrinello, TD-DFT, GW approximation with plane wave and gaussian basis set.
Experience with the codes: Abinit, Quantum-Espresso, DP, Yambo, Gaussian.
Knowledge of the programming languages Fortan, C, Python and of the MPI libraries.
Knowledge of CAD tools used in electronic (SPICE and gate level Power Integrity tools).

ADMINISTRATIVE EXPERIENCES

1. Scientist in charge of 3 user projects of the European Theoretical Spectroscopy Facility with permanent researchers.
2. Principal investigator for 9 supercomputing grant at CINECA (ISCRA class C grants).
3. Referee service for Eur. Phys. J. B.

Data 25/7/2019 Luogo Besana in Brianza