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Codice concorso 4956

Luca Bursi
CURRICULUM VITAE

(N.B. IL CURRICULUM NON DEVE ECCEDERE LE 30 PAGINE E DEVE CONTENERE GLI ELEMENTI CHE IL CANDIDATO RITIENE UTILI AI FINI DELLA VALUTAZIONE.
LE VOCI INSERITE NEL FACSIMILE SONO A TITOLO PURAMENTE ESEMPLIFICATIVO E POSSONO ESSERE SOSTITUITE, MODIFICATE O INTEGRATE)

Curriculum Vitae et Studiorum

March 2022

Luca Bursi, PhD

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PERSONAL INFORMATION

Date of birth: October 23, 1988 Place of birth: Scandiano (RE), Italy
Nationality: Italian Gender: Male

RESEARCH EXPERIENCE

- Aug. 2020 – Current: **Senior Postdoctoral Researcher**
  Institute for Nanoscience, CNR-NANO-S3, via Campi 213/A, 41125, Modena, Italy
  First Principles DFT, Complex Systems, Devices Modeling (INTERSECT EU project)
  Advisor: Dr. Arrigo Calzolari
- Aug. 2020 – Jul. 2021: **Visiting Scholar** on *Catalysis on solvated interfaces*
  Department of Physics, University of North Texas (UNT), Denton, TX 76203, USA
  Advisor: Prof. Oliviero Andreussi
- May 2019 – Jul. 2020: **Postdoctoral Research Associate**
  Department of Physics, University of North Texas (UNT), Denton, TX 76203, USA
  Theoretical Quantum Optics and Implicit Solvation Schemes for Condensed Matter
  Advisor: Prof. Oliviero Andreussi
- May 2017 – May 2019: **Postdoctoral Research Associate**
  Department of Physics and Astronomy & Laboratory for Nanophotonics,
  Rice University, 6100 Main St., Houston, TX 77005, USA
  Theoretical Quantum and Classical Plasmonics and Nanophotonics
  Advisor: Prof. Peter Nordlander
- Oct. 2015 – Feb. 2016: **Visiting Scholar** on *Theoretical Nanophotonics*

Laboratory for Nanophotonics, Rice University, Houston, TX 77005, USA
Advisor: Prof. Peter Nordlander

- Jan. 2014 – Mar. 2017: **PhD student**
  Department of Physics, Informatics and Mathematics, University of Modena and Reggio Emilia & Institute for Nanoscience, CNR-NANO-S3, Modena, Italy
  Theoretical Quantum Nanoplasmonics, Condensed Matter Physics
  Advisors: Prof. Stefano Corni, Dr. Arrigo Calzolari, Prof. Elisa Molinari

EDUCATION

- Mar. 2017: **PhD in Physics and Nano Sciences** (cum Laude)
  Department of Physics, Informatics and Mathematics, University of Modena and Reggio Emilia & Institute for Nanoscience, CNR-NANO-S3, Modena, Italy
  Thesis: Quantifying the plasmonic character of optical excitations at the nanoscale
  Advisors: Prof. Stefano Corni, Dr. Arrigo Calzolari, Prof. Elisa Molinari
- Oct. 2013: **MSc in Physics** (cum Laude)
  University of Modena and Reggio Emilia, Modena, Italy
  Thesis: π-conjugated carbon-based nanosystems: optical excitations and size-effects
  Advisors: Dr. Arrigo Calzolari, Prof. Stefano Corni, Prof. Elisa Molinari
- Oct. 2010: **BSc in Physics** (cum Laude)
  University of Modena and Reggio Emilia, Modena, Italy
  Thesis: First principles investigation of the Cu(111) surface
  Advisors: Dr. Carlo Cavazzoni, Prof. Giorgio Santoro
- May 2010: **Visiting Student** (May – Jul. 2010)
  CINECA Supercomputing Center, Bologna, Italy
  Computational Condensed Matter Physics, MPI/OpenMP Parallel Computing
  Advisor: Dr. Carlo Cavazzoni

RESEARCH INTEREST

My research interest involves the investigation of electronic and optical properties of solid state materials, nanostructures and molecular assemblies, using state-of-the-art *ab initio* density-functional theory (DFT), time-dependent DFT, and beyond; modeling catalytic and electrochemical processes on solvated interfaces by means of state-of-the-art implicit solvation schemes for DFT-based condensed matter simulations; and computational modeling of plasmonic nanostructures through advanced electromagnetic simulation techniques.

Currently, my activity focuses on the development, testing and application of first principles simulations and high-throughput workflows for the study of defective and/or complex systems (e.g., disordered, polycrystalline, amorphous, etc.), in order to improve the modeling and understanding of next-generation devices for synaptic electronics and neuromorphic computing, as part of the European project INTERSECT.

GRANTS AWARDED

- Dec. 2018: 2018 Innovative Collaborative Grant Award
  Department of Nanomedicine, Houston Methodist & Rice University
  Project entitled: *Implantable continuous-mode device for early-stage detection and treatment of inflammation state caused by any implanted foreign body*

- 2013 – 2018: 5 ISCRA Grants for supercomputing resources (4 as PI; 1 as Co-PI)

- 2021 – ongoing: 1 ISCRA Grant for supercomputing resources as PI

SCIENTIFIC PUBLICATIONS AND COMMUNICATIONS

Coauthor of 13 publications on international peer-reviewed journals (2 as first author). Citations: 302 on Google Scholar, 234 on Scopus; h-index: 8 on Google Scholar, 8 on Scopus (Mar. 31st 2022). Author ID on ORCID: http://orcid.org/0000-0002-4530-0424. Author ID on Scopus: 56575141100. Scientific communications include 2 seminars; 10 oral and 13 poster contributions and participation in 20 international conferences; plus 4 oral and 4 poster contributions accepted in 3 international conferences then cancelled in 2020.

BRIEF DESCRIPTION OF RESEARCH ACTIVITY

My research activity focused, during my master thesis and PhD at the **University of Modena and Reggio Emilia and Italian Institute of Nanoscience, CNR-NANO-S3, Modena, Italy**, and under the joint supervision of Prof. Stefano Corni, Dr. Arrigo Calzolari and Prof. Elisa Molinari, on the introduction, development and implementation of original microscopic approaches specifically designed to **quantify the plasmonic character of optical excitations in** (small) **nanostructures**. This involved both the reformulation at the microscopic level of existing concepts, such as the plasmonic electric field enhancement [1], and the introduction of new descriptors, based on rigorous theoretical derivations, called plasmonicity indexes [3,4]. Such approaches provide simple and physically sound tools for the identification of plasmon-like excitations, starting from the simulations of the optical properties of nanosystems. The plasmonicity indexes have been implemented in atomistic *first principles* methods based on time-dependent density-functional theory (TDDFT) [3], spherical jellium descriptions of nanoparticles, and Classical Electrodynamics [4]. They have been applied to analyze the plasmonic behavior of metallic and semiconductor nanoclusters, prototypical C-based molecules, paradigmatic hybrid systems, as well as nanospheres described within the jellium model and larger nanoparticles modeled through classical electrodynamics [3,4]. I performed the first principles DFT and TDDFT simulations on the systems studied with Quantum Espresso (QE) and GAMESS computer codes and I coded the plasmonicity indexes approaches as homemade parallel post-processing tools that exploit directly the outputs of QE and GAMESS. In particular, Ref. [4] was the result of an international collaboration among a few pioneering groups in “quantum” nanoplasmonics: Prof. P. Nordlander’s group at Rice University, Houston, TX, U.S.A., which I visited during my PhD, Prof. F. J. García de Abajo’s group at ICFO, Barcelona Institute of Science and Technology, Barcelona, Spain, E. A. Carter’s group at Princeton University, Princeton, NJ, U.S.A., and my supervisors and me at the University of Modena and Reggio Emilia and CNR-NANO-S3, Modena, Italy.

I continued working on the identification of plasmonic excitations in molecular and ultra-small nanostructures during my postdoc in **Prof. Peter Nordlander’s group** at Rice University, Houston, TX, USA. In collaboration with Prof. Naomi J. Halas’ experimental group, also at Rice University, the **excited-states decay dynamics of molecular plasmons in selected polycyclic aromatic hydrocarbons**, both in their charged and neutral configurations, have been probed with special emphasis on the de-excitation pathways, and we theoretically investigated their collective character [5,10]. I performed the first principles DFT and TDDFT simulations mainly with GAUSSIAN and GAMESS computer codes.

At the same time, under the supervision of Prof. Nordlander and in collaboration with Prof. Alessandro Alabastri and Prof. Stephan Link’s group at Rice University, I used finite element method (FEM) electromagnetic simulations, as implemented in the commercial software COMSOL Multiphysics, to model the **chiroptical response of individual nanoantennas to the polarization states achievable in surface waves**. More specifically, we observed giant modulation of the visible light scattering from gold half-ring and pinwheel nanoantennas excited through total internal reflection of left- and right-handed circularly polarized light, by exploiting the distinct polarization properties of evanescent waves [6]. Such polarization properties were shown to be required for obtaining intense polarization-dependent responses and the FEM electromagnetic simulations agreed very well with experimental measurements. These results provide a fundamentally different mechanism for chiroptical responses requiring a phase delay between transverse and longitudinal electric field oscillations, not found in free-space light, whereas traditional mechanisms of circular dichroism only require structural sensitivity to a relative phase difference between transverse-field oscillations. We then investigated such mechanism more fundamentally when we demonstrated matter’s inherent sensitivity to the direction of the trochoidal field and named this property ***trochoidal dichroism*** [9]. We observed trochoidal dichroism in the differential excitation of bonding and antibonding plasmon modes for a system composed of two coupled dipole scatterers. Trochoidal dichroism constitutes the observation of a geometric basis for polarization sensitivity that fundamentally differs from linear and circular dichroism. It could also be used to characterize molecular systems, such as certain light-harvesting antennas, with cartwheeling charge motion upon excitation.

I also contributed to two projects, in collaboration with Prof. Halas' group at Rice University, where the **bottom-up growths of Al nanocrystals and nanocubes essentially controlled by the choice of the reaction solvent** together with reaction time and temperature were presented [7,8]. In particular, I calculated the first principles optical absorption spectra, at the TDDFT level, of several Ti–Al compounds in different (implicit) solvents, by means of QE and GAUSSIAN codes, which, together with other independent theoretical simulations, supported the experimental finding and conclusions.

More specifically, through careful analysis of the colloidal synthesis of Al nanocrystals (NCRs) through EPR and ^{1}H NMR spectroscopies, a mechanism for the reactions by which **titanium(IV) isopropoxide $Ti(OiPr)_4$ mediates the polymerization of AlH_3 into Al NCRs** has been elucidated, on the one hand. AlH_3 is a single-source precursor for Al metal with hydride oxidation into H_2, catalyzed by $Ti^{3+}(OiPr)_3$, providing the electrons required to produce metallic Al clusters. These clusters are colloidally unstable and coalesce and grow until they reach sufficiently large size to become colloidally stable. This essentially demonstrates a method to tune the size of metallic aluminum NCRs over a 100 nm range by changing the reaction solvent [7].

On the other hand, by decomposing AlH_3 with Tebbe's reagent in tetrahydrofuran, single-crystalline {100} terminated Al nanocubes (NCUs) straightforward colloidal synthesis has been achieved. **The size and shape of the Al NCUs is controlled by the reaction time and the ratio of AlH_3 to Tebbe's reagent**, which, together with reaction temperature, establish kinetic control over Al NCU growth. Al NCUs possess strong localized field enhancements at their sharp corners and resonances highly amenable to coupling with metallic substrates. Their native oxide surface renders them extremely air stable. Chemically synthesized Al NCUs provide an earth-abundant alternative to noble metal NCUs for plasmonics and nanophotonics applications [8].

During my postdoc in **Prof. Oliviero Andreussi's group** at the University of North Texas, Denton, TX, USA, I exploited the state-of-the-art multiscale continuum embedding schemes for first principles condensed matter simulations, as implemented in the Environ plugin of the QE suite of codes, to model catalytical and electrochemical processes on solvated interfaces. I focused, on the one hand, on the **solvation effects in the oxygen evolution reaction (OER) on a promising catalyst such as TiO_2**, whose microscopic mechanism has recently been subject of extensive research. On the other hand, I contributed to the investigation, simulation and **screening of catalytic activities, performances and properties of a database of candidate two-dimensional (2D) materials for OER and oxygen reduction reaction (ORR)** by means of homemade systematic high-throughput workflows exploiting accurate computational thermodynamic approaches, based on first-principles simulations [12].

As a "Senior" postdoc in **Dr. Arrigo Calzolari's group** at the Italian Institute of Nanoscience, CNR-NANO-S3, Modena, Italy I am focusing on the **development**, testing and **application** of scientific computing approaches and **first principles simulations high-throughput workflows** (e.g. based on AiiDA), and on the design and application of multi-scale simulations based on finite element methods and continuous models (e.g. COMSOL Multiphysics) for the study of complex systems (e.g. **defective**, disordered, polycrystalline, **amorphous**, nanostructured, etc.) in order to understand the fundamental operational mechanisms and successfully model devices for synaptic electronics, neuromorphic computation, and more as part of the European project INTERSECT (PI: Dr. Calzolari).

In collaboration with José Vidal-Gancedo's group at the Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Spain, we studied the anchoring of active organic radicals on gold nanoparticles (AuNPs) surface in the context of molecular spintronic devices [13]. In particular, we report the first demonstration of a **surface molecular switch based on AuNPs decorated with persistent perchlorotriphenylmethyl (PTM) radicals**. The redox properties of PTM are exploited to fabricate electrochemical switches with optical and magnetic responses, showing high stability and reversibility. Electronic interaction between the radicals and the gold surface is investigated by UV−vis, showing a very broad absorption band in the near-infrared (NIR) region, which becomes more intense when PTMs are reduced to anionic phase. By using multiple experimental techniques, we demonstrate that this interaction is likely favored by the preferentially flat orientation of PTM ligands on the metallic NP surface, as confirmed by first principles simulations.

PUBLICATIONS LIST

[13] V. Lloveras, P. Elías-Rodríguez, L. Bursi, E. Shirdel, A. R. Goñi, A. Calzolari, J. Vidal-Gancedo. Multifunctional Switch Based on Spin-Labeled Gold Nanoparticles. ***Nano Lett.***, **22** (2), 768−774 (2022). https://doi.org/10.1021/acs.nanolett.1c04294.

[12] N. Karmodak, L. Bursi, O. Andreussi. Oxygen evolution and reduction on two-dimensional transition metal dichalcogenides.
J. Phys. Chem. Lett., **13** (1), 58−65 (2022). https://doi.org/10.1021/acs.jpclett.1c03431.

[11] S. S. E. Collins, E. K. Searles, L. J. Tauzin, M. Lou, L. Bursi, Y. Liu, J. Song, C. Flatebo, R. Baiyasi, Y.-Y. Cai, B.Foerster, T. Lian, P. Nordlander, S. Link, C. F. Landes. Plasmon energy transfer in hybrid nanoantennas.
ACS Nano, **15** (6), 9522–9530 (2021). https://doi.org/10.1021/acsnano.0c08982.

[10] K. D. Chapkin, L. Bursi, B. D. Clark, G. Wu, A. Lauchner, A.-L. Tsai, P. Nordlander, N. J. Halas. Effects of electronic structure on molecular plasmon dynamics.
J. Phys. Chem. C, **124** (37), 20450–20457 (2020). https://doi.org/10.1021/acs.jpcc.0c06072.

[9] L. A. McCarthy, K. W. Smith, X. Lana, S. A. Hosseini Jebeli, L. Bursi, A. Alabastri, W.-S. Chang, P. Nordlander, S. Link. Polarized evanescent waves reveal trochoidal dichroism. ***Proc. Natl. Acad. Sci. USA***, **117** (28), 16143–16148 (2020). https://doi.org/10.1073/pnas.2004169117.

[8] B. D. Clark, C. R. Jacobson, M. Lou, D. Renard, G. Wu, L. Bursi, A. S. Ali, D. F. Swearer, A.-L. Tsai, P. Nordlander, N. J. Halas. Aluminum nanocubes have sharp corners. ***ACS Nano***, **13** (8), 9682–9691 (2019). https://doi.org/10.1021/acsnano.9b05277.

[7] B. D. Clark, C. J. DeSantis, G. Wu, D. Renard, M. J. McClain, L. Bursi, A.-L. Tsai, P. Nordlander, N. J. Halas. Ligand-dependent colloidal stability controls the growth of aluminum nanocrystals. ***J. Am. Chem. Soc.***, **141** (4), 1716–1724 (2019). https://doi.org/10.1021/jacs.8b12255.
[*JACS Spotlights:* ***J. Am. Chem. Soc.***, **141**, 1393–1393 (2019)].

[6] K. W. Smith, L. A. McCarthy, A. Alabastri, L. Bursi, W-S Chang, P. Nordlander, S. Link. Exploiting evanescent field polarization for giant chiroptical modulation from achiral gold half-rings. ***ACS Nano***, **12** (11), 11657–11663 (2018). https://doi.org/10.1021/acsnano.8b07060.

[5] K. D. Chapkin, L. Bursi, G. J. Stec, A. Lauchner, N. J. Hogan, Y. Cui, P. Nordlander, N. J. Halas. Lifetime dynamics of plasmons in the few-atom limit.
Proc. Natl. Acad. Sci. USA, **115** (37), 9134–9139 (2018). https://doi.org/10.1073/pnas.1805357115.

[4] R. Zhang, L. Bursi, J. D. Cox, Y. Cui, C. M. Krauter, A. Alabastri, A. Manjavacas, A. Calzolari, S. Corni, E. Molinari, E. A. Carter, F. J. García de Abajo, H. Zhang, P. Nordlander. How to identify plasmons from the optical response of nanostructures. ***ACS Nano***, **11** (7), 7321–7335 (2017). https://doi.org/10.1021/acsnano.7b03421.

[3] L. Bursi, A. Calzolari, S. Corni, E. Molinari. Quantifying the plasmonic character of optical excitations in nanostructures. ***ACS Photonics***, **3** (4), 520–525 (2016). https://doi.org/10.1021/acsphotonics.5b00688.

[2] F. J. García de Abajo, R. Sapienza, M. Noginov, F. Benz, J. Baumberg, S. Maier, D. Graham, J. Aizpurua, T. Ebbesen, A. Pinchuk, J. Khurgin, K. Matczyszyn, J. T. Hugall, N. van Hulst, P. Dawson, C. Roberts, M. Nielsen, L. Bursi, M. Flatté, J. Yi, O. Hess, N. Engheta, M. Brongersma, V. Podolskiy, V. Shalaev, E. Narimanov, A. Zayats. Plasmonic and new plasmonic materials: general discussion. ***Faraday Discuss.***, **178**, 123–149 (2015). https://doi.org/10.1039/C5FD90022K.

[1] L. Bursi, A. Calzolari, S. Corni, E. Molinari. Light-induced field enhancement in nanoscale systems from first-principles: the case of polyacenes.
ACS Photonics, **1** (10), 1049–1058 (2014). https://doi.org/10.1021/ph500269q.

SELECTED CONTRIBUTIONS IN INTERNATIONAL CONFERENCES

Mar. 2021 L. Bursi, R. Chouhan, A. Catellani, A. Calzolari. *Formation and Diffusion of Charged and Neural Defect States in Crystalline GeSe for Synaptic Electronics.* **2021 APS March Meeting** (Virtual meeting). Oral Presentation.

Jul. 2018	L. Bursi, R. Zhang, K. D. Chapkin, A. Alabastri, N. J. Halas, P. Nordlander. *Universal metric for "plasmonicity" of excitations at the nanoscale*. **Plasmonics and Nanophotonics Gordon Research Conference** (Grand Summit Hotel at Sunday River, Newry, ME, USA). Poster Presentation.
Aug. 2017	L. Bursi, A. Calzolari, S. Corni, E. Molinari, P. Nordlander. *Towards quantitative Quantum Nanoplasmonics*. **Smalley-Curl Institute 3rd Annual Summer Research Colloquium** (Smalley-Curl Institute, Rice University, Houston, TX 77005, USA). Oral Presentation.
Aug. 2016	L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Quantifying the plasmonic character of optical excitations in nanostructures*. **Quantum Plasmonics (QUPLA) Workshop** (Imperial College London, Royal School of Mines, South Kensington, London, UK). Poster Presentation.

MENTORSHIP AND TEACHING

2019	Teaching Assistant (to graduate students) for the Course of Multiphysics Modeling (ESEL 677 002, 26231), ECE Department, Rice University, held by Prof. Alessandro Alabastri (3 credit hours).
2016	Teaching Assistant for the Course of Quantum Mechanics, University of Modena and Reggio Emilia, funded by the Italian Government (35 hrs.).
2014 – 2015	Teaching Assistant (to undergraduate students) for the Course of Quantum Mechanics, University of Modena and Reggio Emilia (70 hrs.).

COMPUTER SKILLS

Programming: Fortran, Python, Matlab, Pascal, C, C++, shell, parallel MPI and OpenMP paradigms (basic level), linear algebra techniques, data fitting.

Scientific software programs: Quantum ESPRESSO, GAMESS, GAUSSIAN and OCTOPUS (*ab initio* simulations); AiiDA (automated, interactive infrastructure and database for simulations); COMSOL Multiphysics (multi-scale, continuous models-based, and classical electromagnetic simulations); Mathematica, Matlab (numerical calculations); gnuplot, grace, Avogadro, VMD (visualization and numerical analysis); etc.

OTHER MERITS

Referee for: Nature Physics, Nature Communications, ACS Nano, Physical Review X, Nanoscale, Chemical Communications, Applied Clay Science, ACS Applied Nano Materials, Physical Review B, Chemical Physics Letters, Molecules, Catalysts, Materials, Sensors, Coatings, Journal of Physics and Chemistry of Solids, The Journal of Physical Chemistry, Applied Sciences, Applied Physics A: Materials Science and Processing.
Publons verified records: https://publons.com/a/1582985; merit: > **90th percentile**.

Good skills in relationship with other people. Experience in teamwork and collaboration. Experience in teaching and educational activities with high school and university students.

MEMBERSHIPS

Material Research Society (2020-2021); American Physical Society (2019–2022).
Italian Society of Chemistry (2018–2019); Royal Society of Chemistry (2015–2016).

REFERENCES

- Arrigo Calzolari, Istituto Nanoscienze-CNR-S3, Modena, Italy arrigo.calzolari@nano.cnr.it
- Stefano Corni, University of Padova, Padova, Italy stefano.corni@unipd.it

- Peter Nordlander, Rice University, Houston, TX, USA nordland@rice.edu
- Oliviero Andreussi, University of North Texas, Denton, TX, USA oliviero.andreussi@unt.edu
- Naomi J. Halas, Rice University, Houston, TX, USA halas@rice.edu
- Elisa Molinari, University of Modena and Reggio Emilia, Italy elisa.molinari@unimore.it

Luca Bursi

Data 31/03/2022 Luogo Modena

Additional Information

ISCRA GRANTS FOR SUPERCOMPUTING RESOURCES AWARDED

6. (Nov 2021 – ongoing) PI for the Iscra C project *First principles characterization of defect states in materials, through AiiDA, QE, and NEB, for next-generation technology* (acronym: AiiDAdef) using the HPC systems MARCONI 100 (IBM Power9 AC922 processors, accelerated with NVIDIA Volta V100 GPUs) and GALILEO 100 (Intel CascadeLake processors) at CINECA Supercomputing Center, Bologna, Italy.

5. (Jul 2017 – Apr 2018) Co-PI for the Iscra C project *Studying the 2D and 1D size-dependence of the GPI by scaling the size of PAHs and Na atomic nanowires, in particular their length and aspect ratio, through TurboTDDFT and PlasmInd-GPI, toward comparison with independent jellium model, RPA and Classical Electrodynamics calculations* (acronym: GPI-Q1D) using the HPC system MARCONI Lenovo NeXtScale (Broadwell processors) and MARCONI Lenovo Adam Pass (Knights Landing processors) at CINECA Supercomputing Center, Bologna, Italy.

4. (Aug 2016 – May 2017) PI for the Iscra C project *Studying the 3D, 2D and 1D size-dependence of the Plasmonicity Index by scaling the size of metal nanoclusters, through TurboTDDFT and PlasmInd, toward comparison with independent jellium model analysis* (acronym: ScalPInd) using the HPC system GALILEO IBM NeXtScale and MARCONI Lenovo NeXtScale at CINECA Supercomputing Center, Bologna, Italy.

3. (Oct 2015 – Jul 2016) PI for the Iscra C project *Characterizing plasmonic properties of graphene nanoflakes through TurboTDDFT and PlasmInd for nanoplasmonic applications* (acronym: PInd-GNF) using the HPC system FERMI Blue Gene/Q and GALILEO IBM NeXtScale at CINECA Supercomputing Center, Bologna, Italy.

2. (Oct 2014 – Jul 2015) PI for the Iscra C project *Testing a Plasmonic Index through TurboTDDFT for nanoplasmonics applications* (acronym: PlasmInd) using the HPC system FERMI Blue Gene/Q at CINECA Supercomputing Center, Bologna, Italy.

1. (Feb 2013 – Dec 2013) PI for the Iscra C project *Evaluating performances and scaling of TurboTDDFT for nanoplasmonics applications* (acronym: TDPlasm) using the HPC system FERMI Blue Gene/Q at CINECA Supercomputing Center, Bologna, Italy.

SEMINARS

Jun. 26, 2017 L. Bursi. *Towards quantitative quantum nanoplasmonics: Strategies to measure the "plasmonicity" of optical excitations in nanostructures*.
Smalley-Curl Institute, Rice University, Houston, TX 77005, USA.

Feb. 1, 2017 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Strategies for the quantification of the plasmonic character of optical excitations in nanostructures*.
CNR-Nano colloquia, Center S3, CNR Institute of Nanoscience, University of Modena and

Reggio Emilia, Modena, Italy.

INTERNATIONAL CONFERENCES AND WORKSHOPS

Nov. 2021 L. Bursi, R. K. Chouhan, A. Catellani, A. Calzolari. *Ab initio characterization of defect states in materials for next-generation technology*. **International Workshop on Advanced Materials-to-Device Solutions for Synaptic Electronics** (Barcelona, Spain). Poster Presentation.

Mar. 2021 L. Bursi, R. K. Chouhan, A. Catellani, A. Calzolari. *Formation and Diffusion of Charged and Neural Defect States in Crystalline GeSe for Synaptic Electronics.* **2021 APS March Meeting** (Virtual meeting). Oral Presentation.

Mar. 2021 L. Bursi, R. Zhang, K. D. Chapkin, N. J. Halas, P. Nordlander. *Universal metric for "plasmonicity" of excitations at the nanoscale*. **2021 APS March Meeting** (Virtual meeting). Poster Presentation.

Mar. 2021 L. Bursi, L. A. McCarthy, K. W. Smith, A. Alabastri, W.-S. Chang, P. Nordlander, S. Link. *Evanescent field polarization for giant chiroptical modulation from achiral gold half-rings: Theoretical insight from simulations*. **2021 APS March Meeting** (Virtual meeting). Poster Presentation.

Nov. 2020 L. Bursi, R. Zhang, K. D. Chapkin, N. J. Halas, P. Nordlander. *Universal metric for "plasmonicity" of excitations at the nanoscale*. **2020 Virtual MRS Spring/Fall Meeting & Exhibit** (Virtual meeting). Oral Presentation.

Nov. 2020 L. Bursi, L. A. McCarthy, K. W. Smith, A. Alabastri, W.-S. Chang, P. Nordlander, S. Link. *Evanescent field polarization for giant chiroptical modulation from achiral gold half-rings: Theoretical insight from simulations*. **2020 Virtual MRS Spring/Fall Meeting & Exhibit** (Virtual meeting). Oral Presentation.

Jul. 2019 L. Bursi, R. Zhang, K. D. Chapkin, N. J. Halas, P. Nordlander. *Universal metric for "plasmonicity" of excitations at the nanoscale*. **ESCOMP 2019: Advanced Electronic Structure Methods in Condensed Matter Physics** (EPFL, Lausanne, Switzerland). Poster Presentation.

Aug. 2018 L. Bursi, R. Zhang, K. D. Chapkin, N. J. Halas, P. Nordlander. *Universal metric for "plasmonicity" of excitations at the nanoscale*. **Smalley-Curl Institute 4th Annual Summer Research Colloquium** (Smalley-Curl Institute, Rice University, Houston, TX 77005, USA). Oral Presentation.

Jul. 2018 L. Bursi, R. Zhang, K. D. Chapkin, A. Alabastri, N. J. Halas, P. Nordlander. *Universal metric for "plasmonicity" of excitations at the nanoscale*. **Plasmonics and Nanophotonics Gordon Research Conference** (Grand Summit Hotel at Sunday River, Newry, ME, USA). Poster Presentation.

Aug. 2017 L. Bursi, A. Calzolari, S. Corni, E. Molinari, P. Nordlander. *Towards quantitative Quantum Nanoplasmonics*. **Smalley-Curl Institute 3rd Annual Summer Research Colloquium** (Smalley-Curl Institute, Rice University, Houston, TX 77005, USA). Oral Presentation.

Aug. 2016 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Quantifying the plasmonic character of optical excitations in nanostructures*. **Quantum Plasmonics (QUPLA) Workshop** (Imperial College London, Royal School of Mines, South Kensington, London, UK). Poster Presentation.

Jul. 2016 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Towards a quantitative description of the plasmonic character of optical excitations in nanostructures*. **META 2016, the 7th International Conference on Metamaterials, Photonic Crystals and Plasmonics** (Torremolinos, Malaga, Spain). Oral Presentation.

Jun. 2016 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Light-induced field enhancement in polyacenes*. **SINFO - Surface, Interface and Functionalization Processes in Organic Compounds**

and Applications - 3rd Workshop (University Federico II of Naples, Italy). Poster Presentation.

Apr. 2016 Participation in the **Nanostructured Metal Optics: from Theory to Enhanced Spectroscopies, Sensing, Imaging Workshop** (Scuola Normale di Pisa, Italy).

Jul. 2015 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Quantifying the plasmonic character of optical excitations in nanostructures from first principles*. **Plasmonica 2015 Workshop** (University of Padua, Italy). Oral Presentation.

Mar. 2015 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Light-induced field enhancement in polyacenes*. **DPG Spring Meeting** (Technische Universitaet, Berlin, Germany). Oral Presentation.

Feb. 2015 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Light-induced field enhancement in polyacenes*. **Nanomaterials for Applications in Energy Technology Gordon Research Conference** (Ventura Beach Marriott, Ventura, CA, USA). Poster Presentation.

Feb. 2015 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Light-induced field enhancement in polyacenes*. **Nanomaterials for Applications in Energy Technology Gordon Research Seminar** (Ventura Beach Marriott, Ventura, CA, USA). Poster Presentation.

Feb. 2015 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Light-induced field enhancement in polyacenes*. **Nanomaterials for Applications in Energy Technology Gordon Research Seminar** (Ventura Beach Marriott, Ventura, CA, USA). Oral Presentation.

Feb. 2015 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Light-induced field enhancement in polyacenes*. **Faraday Discussion 178: Nanoplasmonics** (Royal Society of Chemistry at Burlington House and Geological Society, London, UK). Poster Presentation.

Jan. 2015 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Light-induced field enhancement in polyacenes*. **International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods** (International Centre for Theoretical Physics, Trieste, Italy). Poster Presentation.

Jul. 2014 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Light-induced field enhancement in polyacenes*. **Plasmonica 2014 Workshop** (University of Rome Sapienza, Italy). Poster Presentation.

Jun. 2014 L. Bursi, A. Calzolari, S. Corni, E. Molinari. *Light-induced field enhancement in polyacenes*. **SINFO - Surface, Interface and Functionalization Processes in Organic Compounds and Applications - 2nd Workshop** (University of Trieste, Italy). Oral Presentation.

Nov. 2013 Participation in the **Conference on Frontiers of Condensed Matter Physics** (International Centre for Theoretical Physics, Trieste, Italy).

SCIENTIFIC SCHOOLS

Jun. 2014 ICOE 2014 School on Predictive Modelling and Computational Methods for Organic Electronics (University of Modena and Reggio Emilia, Italy).

Mar. 2013 Introduction to the FERMI Blue Gene/Q for users and developers (CINECA Supercomputing center, Bologna, Italy).

Aug. 2012 HoW exciting! Hands-on Workshop on Excitations in Solids 2012 (Humboldt Universitaet zu Berlin, Germany).

Jun. 2010 Summer School on Parallel Computing (CINECA Supercomputing center, Bologna, Italy).

Jun. 2010 Introduction to the Blue Gene/P for users and developers (CINECA Supercomputing center, Bologna, Italy).

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