Curriculum Vitae et Studiorum

April 2020

Luca Bursi, PhD

Department of Physics, University of North Texas (UNT),
1155 Union Cir., Denton, TX 76203, USA

Academic visitor, Department of Physics and Astronomy & Laboratory for Nanophotonics,
Rice University, 6100 Main St., Houston, TX 77005, USA

PERSONAL INFORMATION

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

RESEARCH EXPERIENCE

- May 2019 – Current: **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 of 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 of 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

Denton, Texas, U.S.A., 24 / 04 / 2020

- 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

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)

SCIENTIFIC PUBLICATIONS AND COMMUNICATIONS

Coauthor of 8 publications on international peer-reviewed journals (2 as first author). Citations: 131 on Google Scholar, 106 on Scopus; h-index: 6 on Google Scholar, 5 on Scopus (April 24th 2020). Author ID on ORCID: http://orcid.org/0000-0002-4530-0424. Author ID on Scopus: 56575141100. Scientific communications include 2 seminars, 7 oral and 10 poster contributions in 18 international conferences.

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, 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 home-made parallel post-processing tools that exploit directly the outputs of QE and GAMESS. In particular, the work published in 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 in such occasion for four months 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 two years postdoc in Prof. Nordlander's group at Rice University. In particular, in collaboration with Prof. N. 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 de-excitation pathways, and we theoretically investigated their collective character [5]. I performed the first principles DFT and TDDFT simulations mainly with GAUSSIAN and GAMESS computer codes. A follow-up work along this research line will be soon submitted for publication.

At the same time, under the supervision of Prof. A. Alabastri and Prof. Nordlander and in collaboration with experimentalists in Prof. S. 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 particular 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. Another more fundamental work focused on this mechanism will appear on *Proc. Natl. Acad. Sci. USA* (2020).

I also contributed to two projects, in collaboration with experimentalists from 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, firstly, 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. 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].

Secondly, by decomposing AlH_3 with Tebbe's reagent in tetrahydrofuran, single-crystalline {100} terminated Al nanocubes (NCUs) straightforward colloidal synthesis have 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. Andreussi's group at the University of North Texas, Denton, TX, U.S.A., I am currently exploiting 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. In particular, I am focusing, on the one hand, on the solvation effects in the oxygen evolution reaction on a promising catalyst such as TiO_2, whose microscopic mechanism has recently been subject of extensive research. On the other hand, I am contributing to design and utilize workflows for the systematic high-throughput simulations and screen of catalytic activity and properties of a database of candidate 2D compounds. I am also contributing to the development and testing of the Environ code.

PUBLICATIONS LIST

[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**, 9682–9691, (2019).

[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**, 1716–1724 (2019). [*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**, 11657–11663 (2018).

[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**, 9134–9139 (2018).

[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**, 7321–7335 (2017).

[3] L. Bursi, A. Calzolari, S. Corni, E. Molinari. Quantifying the plasmonic character of optical excitations in nanostructures. ***ACS Photonics***, **3**, 520–525 (2016).

[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).

[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**, 1049–1058 (2014).

SELECTED CONTRIBUTIONS IN INTERNATIONAL CONFERENCES

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.

MENTHORSHIP 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 and Environ, GAMESS, GAUSSIAN and OCTOPUS (*ab initio* simulations), COMSOL Multiphysics (classical electromagnetic simulations), Mathematica, Matlab (numerical calculations), gnuplot, xmgrace, Avogadro, VMD (visualization and numerical analysis).

OTHER MERITS

Referee of the following journals: Physical Review B, ACS Nano, Nature Physics, Nanoscale, Physical Review X, Chemical Communications, Chemical Physics Letters, Materials, Sensors, Coatings, Applied Sciences, Journal of Physics and Chemistry of Solids.
Publons verified records: https://publons.com/a/1582985.

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

American Physical Society since 2019.

REFERENCES

- Oliviero Andreussi, University of North Texas, Denton, TX, USA oliviero.andreussi@unt.edu
- Peter Nordlander, Rice University, Houston, TX, USA nordland@rice.edu
- Naomi J. Halas, Rice University, Houston, TX, USA halas@rice.edu
- Stefano Corni, University of Padova, Padova, Italy stefano.corni@unipd.it
- Arrigo Calzolari, Istituto Nanoscienze-CNR-S3, Modena, Italy arrigo.calzolari@nano.cnr.it
- Elisa Molinari, University of Modena and Reggio Emilia, Italy elisa.molinari@unimore.it

Additional Information

ISCRA GRANTS FOR SUPERCOMPUTING RESOURCES AWARDED

5. (July 2017 – April 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), CINECA Supercomputing Center, Bologna, Italy

4. (August 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, CINECA Supercomputing Center, Bologna, Italy

3. (October 2015 – July 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, CINECA Supercomputing Center, Bologna, Italy

2. (October 2014 – July 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, CINECA Supercomputing Center, Bologna, Italy

1. (February 2013 – December 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, CINECA Supercomputing Center, Bologna, Italy

SEMINARS

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.

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.

INTERNATIONAL CONFERENCES AND WORKSHOPS

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).