PERSONAL INFORMATION

Claudia Caddeo

Date of birth: 23/12/1982

Place of birth: Iglesias (CI) - Italy

BIBLIOMETRIC INDICATORS

h-index : **13** (Scopus)
total number of citations: **526** (Scopus)
total number of published works: **29** (20 from 2016)

RESEARCH EXPERIENCES

30 Jul 2020 - present

Staff Researcher (permanent position)

Consiglio Nazionale delle Ricerche - IOM Cagliari (CA), Italy

- Research activity: multiscale modeling of polymer and organic blends for photovoltaics; development of novel force fields for hybrid and organic materials;

Business or sector Research

01 Apr 2016 – 31 Dec 2019

Postdoctoral researcher (assegno di ricerca **IOM AR 002/2016 CA**)

Consiglio Nazionale delle Ricerche - IOM Cagliari (CA), Italy

- Research activity on hybrid perovskites for energy applications (photovoltaic, thermoelectric).

Business or sector Research

01 Apr 2015 - 31 Mar 2016

Postdoctoral researcher (assegno di ricerca)

Università Cattolica del Sacro Cuore - Brescia (BS), Italy

- Research activity on ultrafast thermodynamics at the nano-scale. The research activity has been carried out in the framework of FIRB “ULTRANANO” project.

Business or sector Research

02 Jan 2014 - 28 Feb 2015

Postdoctoral researcher (assegno di ricerca e borsa di ricerca)

Università degli Studi di Cagliari (CA), Italy

- Research activity: atomistic study of nanocrystals for hydrogen production from solar energy through photocatalysis. The research activity has been carried out in the framework of the project “Nanocristalli per la produzione di idrogeno dall’energia solare”, financially supported by Regione Autonoma della Sardegna.

Business or sector Research

15 May 2013 - 01 Jan 2014

Postdoctoral researcher (assegno di ricerca)

Consiglio Nazionale delle Ricerche - IOM Cagliari (CA), Italy

- Research activity: multiscale modeling of polymer-based hybrid interfaces and nanostructures. The research activity has been carried out in the framework of IIT SEED project “Polyphemo”.

Business or sector Research

03 May 2010 - 02 May 2013

PhD course (see “Education”)

Università degli Studi di Cagliari (CA), Italy

- The research activity has been carried out in the framework of IIT SEED project “Polyphemo”.

Business or sector Research

01 Feb 2011 - 28 Feb 2011

Graduate researcher (contratto di collaborazione)

Consiglio Nazionale delle Ricerche - IOM Cagliari (CA), Italy

- Research activity: study of the adhesion of polymer chains on carbon nanotubes

Business or sector Research

01 Oct 2009 - 31 Jan 2010

Graduate researcher (contratto co.co.co.)

Consorzio COSMOLAB - CYBERSAR project (http://www.cybersar.com/), Cagliari (CA), Italy

- Research activity: code optimization for molecular dynamics simulations

Business or sector Research

01 Oct 2008 - 31 Mar 2009

Undergraduate researcher

CNES – Centre National d'Études Spatiales, Toulouse, France

- Research activity: Study of the reliability of optoelectronic devices for space applications

Business or sector Research / Space sector

TEACHING EXPERIENCES

Post-graduate courses

11-12 Jan 2018: Lecturer of the **PhD** course “Understanding materials by molecular dynamics simulations: theory and examples” in the framework of the **International Doctoral Program** in Science - Università Cattolica del Sacro Cuore, Brescia (Italy)

26-30 Nov 2012: Lecturer at “School on Numerical Methods for Materials Science Related to Renewable Energy Applications”, Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste (TS), Italy.

University courses

Apr 2010 – Sep 2010 : Teaching assistant for **BSc** course in Electronics Engineering, Università degli Studi di Cagliari (CA), Italy

Mar 2008 - Sept 2008: Teaching assistant for **BSc** course in Electronics Engineering, Università degli Studi di Cagliari (CA), Italy

RESEARCH HIGHLIGHTS

Publications in international peer-reviewed journals

Ben Dkhil, S. , Perkhun, P., Luo, C., ..., **Caddeo C.**, … ,Videlot-Ackermann, C. “Direct Correlation of Nanoscale Morphology and Device Performance to Study Photocurrent Generation in Donor-Enriched Phases of Polymer Solar Cells” ; ACS Applied Materials and Interfaces, 2020, 12(25), pp. 28404-28415. **IF 8.758, Q1**

Mattoni, A., **Caddeo, C.** “Dielectric function of hybrid perovskites at finite temperature investigated by classical molecular dynamics”; Journal of Chemical Physics, 2020, 152(10), 104705. **IF 2.991, Q2**

Caddeo, C., Filippetti, A., Mattoni, A. “The dominant role of surfaces in the hysteretic behavior of hybrid perovskites” ; Nano Energy, 2020, 67, 104162. **IF 16.602, Q1**

Filippetti A., **Caddeo C.**, Bosin A., Delugas P., Mattoni A. “Donuts and Spin Vortices at the Fermi Surfaces of Hybrid Lead-Iodide CH3NH3PbI3 Perovskites”; The Journal of Physical Chemistry C, 2019, 123, 11, 6753-6762. **IF 4.484, Q1**

Caddeo C., Marongiu D., Meloni S., Filippetti A., Quochi F., Saba M., Mattoni A. “Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide”; Advanced Materials Interfaces, 2019, 6(3), 1801173, **IF 4.834, Q1**

Benetti G., Gandolfi, M., Van Bael M. J., Gavioli L., Giannetti C., **Caddeo C.**, Banfi F. “Photoacoustic Sensing of Trapped Fluids in Nanoporous Thin Films: Device Engineering and Sensing Scheme”; ACS applied materials and interfaces, 2018, 10 (33), pp 27947-27954. **IF 8.097, Q1**

Caddeo C., Saba M.I., Meloni S., Filippetti A., Mattoni A. “Collective Molecular Mechanisms in the CH3NH3PbI3 Dissolution by Liquid Water”; ACS Nano, 2017, 11 (9), pp 9183-9190. **IF 13.709, Q1**

Benetti G., **Caddeo C.**, Melis C., Ferrini G., Giannetti C., Winckelmans N., Bals S., Van Bael M. J., Cavaliere E., Gavioli L., Banfi F. “Bottom-Up Mechanical Nanometrology of Granular Ag Nanoparticles Thin Films”; The Journal of Physical Chemistry C, 2017, 121 (40), pp 22434-22441. **IF 4.484, Q1**

Genovese C., Antidormi A., Dettori R., **Caddeo C.**, Mattoni A., Colombo L., Melis C. “Linking morphology to thermal conductivity in PEDOT: an atomistic investigation”; Journal of Physics D: Applied Physics, 2017, 50 (49), pp. **IF 2.373, Q2**

Hata T., Giorgi G., Yamashita K., **Caddeo C.**, Mattoni A. “Development of a Classical Interatomic Potential for MAPbBr3”; The Journal of Physical Chemistry C, 2017, 121 (7), pp 3724-3733. **IF 4.484, Q1**

Filippetti A., **Caddeo C.**, Delugas P. D., Mattoni A. “Photoluminescence, optical gain, and lasing threshold in CH 3 NH 3 PbI 3 methylammonium lead-halide perovskites obtained by ab initio calculations”; Journal of Materials Chemistry C, 2017, 48, 12758-12768. **IF 5.976, Q1**

Caddeo C., Melis C., Ronchi A., Giannetti C., Ferrini G., Rurali R., Colombo L., Banfi F. "Thermal boundary resistance from transient nanocalorimetry: A multiscale modeling approach”; Physical Review B, 2017,95(8),085306. **IF 3.813, Q2**

Filippetti A, **Caddeo C,** Delugas PD, Mattoni A "Appealing Perspectives of Hybrid Lead-Iodide Perovskites as Thermoelectric Materials"; The Journal of Physical Chemistry C, 2016, 120 (50), pp 28472–28479. **IF 4.484, Q1**

Mattoni A, Filippetti A, **Caddeo C** "Modeling hybrid perovskites by molecular dynamics" Journal of Physics: Condensed Matter, 2016 , Volume 29, Number 4. **IF 2.617, Q2**

C. Caddeo, C. Melis, M. I. Saba, L. Colombo, A. Mattoni; “Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure”; Phys. Chem. Chem. Phys., 2016, 18 (35), 24318-24324. **IF 3.906, Q1**

A. Filippetti, A. Mattoni, **C. Caddeo**, M.I. Saba,and P. Delugas; “Low electron-polar optical phonon scattering as a fundamental aspect of carrier mobility in methylammonium lead halide CH3NH3PbI3 perovskites”; Phys. Chem. Chem. Phys.,18, 15352-15362 (2016). **IF 3.906, Q1**

P. Delugas, **C. Caddeo**, A. Filippetti, A. Mattoni; “Thermally Activated Point-Defects Diffusion in Methylammonium Lead Trihalide: Anisotropic and Ultra-High Mobility of Iodine”, J. Phys. Chem. Lett., 7, pp 2356-2361 (2016). **IF 8.709, Q1**

A. Mattoni, A. Filippetti, M.I. Saba, **C. Caddeo** and P. Delugas; “Temperature evolution of methylammonium trihalide vibrations at the atomic scale”, J. Phys. Chem. Lett. 7, 529-535 (2016). **IF 8.709, Q1**

C. Caddeo, V. Calzia, L. Bagolini, M.T. Lusk, A. Mattoni; “Pinpointing the Cause of Platinum Tipping on CdS Nanorods”, J. Phys. Chem. C 119, 22663-22668 (2015). **IF 4.484, Q1**

Bellani, S., Porro, M., **Caddeo**, C., Saba, M.I., Miranda, P.B., Mattoni, A., Lanzani, G., Antognazza, M.R.; “The study of polythiophene/water interfaces by sum-frequency generation spectroscopy and molecular dynamics simulations”, J. Mater. Chem. B 3, Issue 31, 6429-6438 (2015). **IF 4.776, Q1**

C. Caddeo, D. Fazzi, M. Caironi and A. Mattoni; “Atomistic simulations of P(NDI2OD-T2) morphologies: From single chain to condensed phases”, J. Phys. Chem. B 118, 12556-12565 (2014). **IF 3.146, Q2**

C. Caddeo, A. Mattoni; “Atomistic Investigation of the Solubility of 3-Alkylthiophene Polymers in Tetrahydrofuran Solvent”, Macromolecules 46 (19), 8003-8008 (2013). **IF 5.914, Q1**

C. Caddeo, G. Malloci, F. De Angelis, L. Colombo, A. Mattoni; “Optoelectronic properties of (ZnO)60 isomers”, Phys. Chem. Chem. Phys. 14, 14293-14298 (2012). **IF 3.906, Q1**

C. Caddeo, G. Malloci, G.M. Rignanese, L. Colombo, A. Mattoni; “Electronic properties of hybrid zinc oxide-oligothiophenes nanostructures”, J. Phys. Chem. C 116, 8174-8180 (2012). **IF 4.484, Q1**

C. Caddeo, R. Dessì, C. Melis, L. Colombo, A. Mattoni; “Poly(3-hexylthiophene) adhesion on zinc oxide nanoneedles", J. Phys. Chem. C 115, 16833-16837 (2011). **IF 4.484, Q1**

C. Caddeo, C. Melis, L. Colombo, A. Mattoni; “Understanding the helical wrapping of Poly(3-hexylthiophene) on carbon nanotubes”, J. Phys. Chem. C 114, 21109-21113(2010). **IF 4.484,Q1**

P. Spezzigu, **C. Caddeo**, G. Quadri, O. Gilard, L. Bechou, Y. Ousten, M. Vanzi; “Implementation of a "design of Experiments" Methodology for the Prediction of Phototransistor Degradation in a Space Environment”, IEEE Transactions on Nuclear Science 56, 2465-2472 (2009). **IF 1.44, Q1**

Book Chapters

Mattoni A., Filippetti A., **Caddeo C**, "Structural and thermodynamical properties of hybrid perovskites by classical molecular dynamics", Chapter 1 of "Theoretical Modeling of Mixed Organic-Inorganic Perovskites for Photovoltaic Applications", CRC press Taylor and Francis group, ISBN 9781498750783

Caddeo C, Mattoni A, Filippetti A. "Intrinsic electronic, optical and recombination properties described by the density functional theory calculations", Chapter 2 of "Theoretical Modeling of Mixed Organic-Inorganic Perovskites for Photovoltaic Applications", CRC press Taylor and Francis group, ISBN 9781498750783

Contributions to international Conferences

“Hydrophilicity, dissolution and water contact angle on methylammonium lead iodide”, oral contribution, Theory and Computation of Halide Perovskites (ComPer). 8-9 Sept 2020, Online

“Ultrastable PTB7-based organic solar cells investigated by atomistic simulations”, oral contribution, FisMat 2017, 1-5 Oct 2017, Trieste (TS), Italy

“Atomistic study of semiconducting polymers in solvents via Flory-Huggins theory”, oral contribution, materials.it conference, 12-16 December 2016, Catania, Italy

"Calculating phonon interface thermal resistance at metal/oxide interfaces”, poster; CECAM Hot Nanostructures, 30 Sep - 2 Oct 2015, Mainz, Germany

“Atomistic investigation of P(NDI2OD-T2) copolymer in solvents through optimized torsional force field”, oral contribution; E-MRS Spring Meeting 2014, 26-30 May 2014, Lille, France

“Flory-Huggins theory applied to atomistic study of oligo(3-alkylthiophene)s solubility in tetrahydrofuran”, oral contribution; E-MRS Spring Meeting 2014, 26-30 May 2014, Lille, France

"Atomistic investigation of the solubility of (3-alkylthiophene) polymers in tetrahydrofuran solvent", oral contribution; FisMat 2013, 9-13 Sep 2013, Milano (MI), Italy

"Wrapping phenomena in polymer-based hybrids for photovoltaics", poster; CECAM Energy from the Sun, 10-14 Sep 2012, Chia Laguna (CA), Italy

"Nanoscale effects on polymer-ZnO hybrids for photovoltaics", oral contribution; NANOSEA 2012, 25-29 Jun 2012, S. Margherita di Pula (CA), Italy

"Understanding polymer wrapping on rod-like nanostructures", oral contribution; E-MRS Fall Meeting 2011, 19-23 Sep 2011, Warsaw, Poland

"Computer-based design of hybrid nanomaterials for photovoltaics", poster ; ISROS 2010 – International Symposium on Reliability of Optoelectronics in Space, 28-30 Apr 2010, Cagliari (CA), Italy

"Defect characterization in irradiated silicon photodiodes", oral contribution;ISROS 2010 – International Symposium on Reliability of Optoelectronics in Space, 28-30 Apr 2010, Cagliari (CA), Italy

"Evaluation of commercial silicon based photodiode arrays for optical angular encoders", poster; ISROS 2009– International Symposium on Reliability of Optoelectronics in Space, 11-14 May 2009, Cagliari (CA), Italy

Schools and workshops

29 Aug - 09 Sep 2011: *Scuola Estiva di Calcolo Avanzato" (Summer school on advanced computing)* VII edition, organized by CASPUR (Consorzio Interuniversitario per le Applicazioni di Supercalcolo per Università e Ricerca), Grottaferrata (RM), Italy

05 Jul - 23 Jul 2010: "*Summer school on atomistic simulation techniques for material science, nanotechnology and biophysics*", organized by International School for Advanced Studies (SISSA) e Democritos Modeling Center for Research in Atomistic Simulation, Trieste (TS), Italy

Scientific projects (as Principal Investigator)

Oct 2019 - Jul 2020: Principal Investigator of ISCRA supercomputing project "MIxing Ternary Organic MAterials for Solar Cells" (MITOMASC). The project aimed at performing preliminary studies of the miscibility of organic donors (PTB7, PTB7-th and Si-PCPDTBT) and acceptors (PC71BM) of interest for ternary solar cells. The main outcomes of this project are reported in detail in the publication "Direct Correlation of Nanoscale Morphology and Device Performance to Study Photocurrent Generation in Donor-Enriched Phases of Polymer Solar Cells" ; ACS Applied Materials and Interfaces, 2020, 12(25), pp. 28404-28415, and in a paper which has been submitted for publication very recently to Nano Energy (title: "Theoretical insight on PTB7:PC71BM, PTB7-th:PC71BM and Si-PCPDTBT:PC71BM interactions governing blend nanoscale morphology for efficient solar cells").

Jul 2016 – April 2017: Principal Investigator of ISCRA supercomputing project "THErmal conductivity of HYbrid PErovskites" (THEHYPE). The project aimed at investigating the thermal properties of hybrid perovskites for thermoelectric applications.1, 2 and 3D models have been realized and the thermal conductivity κ has been calculated. We have found a very low thermal conductivity in pristine CH3NH3PbI3, and we have determined an optimum doping level for a promising use of hybrid perovskites for thermoelectric applications. The main outcomes of this project are reported in detail in our publications "On the Appealing Perspectives of Hybrid Lead-Iodide Perovskites as Thermoelectric Materials"; The Journal of Physical Chemistry C, 2016, 120 (50), pp 28472–28479, and "Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure"; Phys. Chem. Chem. Phys., 2016, 18 (35), 24318-24324.

Nov 2014 - Aug 2015: Principal Investigator of ISCRA supercomputing project "Theoretical Investigation of Platinum Tipping on cAdmiumsulphide for Photocatalysis" (TIPTAP). Within this project, we have identified the precise mechanism by which metallic platinum aggregates at the tips of cadmium sulfide (CdS) nanostructures. We have simulated physically realistic nanorods and quantified the chemical, dispersive and electrostatic contributions to platinum interaction with CdS. Crystallographic anisotropy as well as facet, edge and tip effects were accounted for to show that Pt aggregation, known as "tipping", is not due to the dynamics of adhesion and diffusion. Instead, efficient tipping is found to be due to long-range electrostatic interactions of metallic ions with polar tips set up by CdS surface stoichiometry. The main outcomes of this work are collected in "Pinpointing the Cause of Platinum Tipping on CdS Nanorods", J. Phys. Chem. C 119, 22663-22668 (2015)

Feb - Nov 2014 : Principal Investigator of ISCRA supercomputing project “Solubility of conductive Polymers in Aromatic Solvents by atomistic Simulations” (SPASS). Within this project, we were able to study the structure, crystallinity, and solubility of a high-mobility n-type semiconducting copolymer, P(NDI2OD-T2) by an atomistic investigation based on model potential molecular dynamics (NAMD code). We have proposed a set of new force field parameters, which have been reparametrized against density functional theory (DFT) calculations, with the aim to reproduce the correct torsional angles that govern the polymer chain flexibility and morphology. We have simulated P(NDI2OD-T2) oligomers in different environments, namely, in vacuo, in the bulk phase, and in liquid toluene and chloronaphthalene solution. Different morphologies and dynamics of the oligomers in the two solvents have been observed, in agreement with experimental findings. The main outcomes of this work are collected in " Atomistic Simulations of P(NDI2OD-T2) Morphologies: From Single Chain to Condensed Phases”, J. Phys. Chem. B 118, 12556-12565 (2014).

Mar - Dec 2013 : Principal Investigator of ISCRA supercomputing project “Atomistic investigation of the Selective WrappIng of carbon Nanotubes by conjuGated polymers in solvents" (SWING). We were able to study the solubility properties of regioregular oligo(3-alkylthiophene)s in tetrahydrofuran solvent as a function of their alkyl chains length. We have used the Flory-Huggins theory, which we have applied for the first time to study the solubility of conjugated conducting polymers in a typical organic solvent. The properties of the isolated solvent and polymer have been correctly reproduced, and the calculated solubilities of the oligo(3-alkylthiophene)s in tetrahydrofuran are in agreement with available experimental data. The methodology applied has proven to be a powerful tool to study the solubility of alkylthiophenes in molecular solvents. The main outcomes of this work are collected in “Atomistic Investigation of the Solubility of 3-Alkylthiophene Polymers in Tetrahydrofuran Solvent”, Macromolecules 46 (19), 8003-8008 (2013)

Dec 2012 - Mar 2013 : Principal Investigator of ISCRA supercomputing project ZINC3HT. Within this project we have studied the adhesion of poly-(3-alkylthiophene) chains on ZnO nanostructures. The latter (nanoneedles) had realistic sizes and were studied by model potential molecular dynamics. The main outcomes of this project are collected in in “Poly(3-hexylthiophene) adhesion on zinc oxide nanoneedles”, J. Phys. Chem. C 115, 16833-16837 (2011).

STUDENT SUPERVISING

Jul 2015 — Co-advisor of BSc thesis in Physics. Thesis title “ Teoria elementare del fenomeno di rettificazione termica in sistemi a stato solido” (Basic theory of thermal rectification in solid state systems), Università degli Studi di Cagliari (CA), Italy.

PUBLIC OUTREACH

11 Feb 2019 — Participation to UNESCO “International day of Women and Girls in Science” initiative

25 Sep 2015 — Participation to “European Researchers’ Night” initiative

26 Sep 2014 — Participation to “European Researchers’ Night” initiative

EDUCATION AND TRAINING

05 Jun 2013

PhD in Physics

Università degli studi di Cagliari (CA), Italy

- Thesis title “Low dimension polymer-based nanostructures for photovoltaics”; advisors Prof. Luciano Colombo and Dr. Alessandro Mattoni.

28 Apr 2009

MSc in Electronics Engineering

110/110 magna cum laude

Università degli studi di Cagliari (CA), Italy

- Thesis title “Analysis of the reliability of optoelectronic devices for space applications”; advisors Prof. Massimo Vanzi and Dr. Gianandrea Quadri.

Sep 2006 - Sep 2007

ERASMUS student

Universidad Miguel Hernandez, Elche (AL), Spain

- Visiting student in the framework of European ERASMUS program

24 Oct 2005

BSc in Electronics Engineering

104/110

Università degli studi di Cagliari (CA), Italy

Sept 2001- Sept 2002

First year of Management Engineering B.Sc.

Politecnico di Milano (MI), Italy

Jul 2001

High school diploma (maturità scientifica)

100/100

Liceo Scientifico G. Asproni, Iglesias (CI), Italy

PERSONAL SKILLS

Mother tongue(s): Italian

Other language(s)	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C1	C1	C1	C1	C1
	Computer-based TOEFL (June 2002) - scored 230/300				
English	C1 – Certificate issued on June 2019 by “Welcome school s.a.s.”				
Spanish	C1	C1	C1	C1	C1
French	B2	B2	B2	B2	B1

Levels: A1/2: Basic user - B1/2: Independent user - C1/2 Proficient user
Common European Framework of Reference for Languages

Computer skills

- good command of LaTex and Microsoft Office™ tools
- good command of Linux, Windows, Mac OS
- good command of scripting languages bash and awk
- good command of simulation codes DL POLY, LAMMPS, Turbomole, NAMD
- good command of visualization software VMD
- good command of programming languages Fortran and C

Other

▪ Peer- reviewing activity for international journals

ACS Nano, ISSN 1936-0851
Materials Today Energy, ISSN 2468-6069
J. Sulf. Chem, ISSN 1741-5993 (Print), 1741-6000 (Online)
Phys. Chem. Chem. Phys., ISSN 1463-9076
Computational Materials Science, ISSN 0927-0256
J. Phys. Chem. C, ISSN 1932-7447 (Print), 1932-7455 (Online)
Solid State Sciences, ISSN 1293-2558 (Print), 1873-3085 (Online)

▪ Development and maintenance of software projects for polymer modeling (POLY2MD code)

Dichiarazione sostitutiva di certificazioni
(Art.46 del D.P.R. 28 dicembre 2000, n. 445)

Dichiarazione sostitutiva dell'atto di notorietà
(Art. 47 del D.P.R. 28 dicembre 2000, n. 445)

La sottoscritta Claudia Caddeo nata a Iglesias (CI) il 23/12/1982, residente in Cagliari (CA) e domiciliata in Cagliari (CA) via Giardini n° 100, a conoscenza di quanto prescritto dall'art. 76 del D.P.R. 28 dicembre 2000, n. 445, sulla responsabilità penale cui può andare incontro in caso di falsità in atti e di dichiarazioni mendaci, ai sensi e per gli effetti del citato D.P.R. n. 445/2000 e sotto la propria personale responsabilità:

D I C H I A R A

che quanto affermato e riportato nel curriculum corrisponde al vero.

Letto, confermato e sottoscritto.

LA DICHIARANTE

_____, li _____ _____