

PERSONAL
INFORMATION

Alessandro Mattoni



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ResearchID: B-7428-2015

Sesso M | Data di nascita 28/02/1972 | Nazionalità Italiana

POSITION
since 15-10-2020 to date

RESEARCH DIRECTOR

National Council of Research, Institute of Materials, Unit of Cagliari

APPOINTMENT
since 01-04-2018 to date

Person in charge of the Unit of Cagliari of Institute of Materials

National Council of Research

SYNOPTIC TABLE
A. MATTONI

RESEARCH ACTIVITY	GRANTS and FUNDING (since 2010)	MANAGEMENT EXPERIENCE	SCIENTIFIC PUBLICATIONS	BIBLIOMETRIC INDECES June 2020 (Scopus)
Multiscale modeling of hybrid nanomaterials for energy, opto- and nano-electronics	<p>> 1Meuro (including ongoing projects)</p> <p>~70 MILLION core HOURS on High Performance Computing infrastructures</p>	<p>Head of research team</p> <p>1<=personnel units<=5</p> <p>person in charge of Unit of Cagliari Institute of Materials IOM-CA</p>	<p>98 publications</p>	<ul style="list-style-type: none"> • H=27 • total citations >2265 • citations/item ~23 • 6 highly cited papers during 2017-2020 (ISI)

HIGHLIGHTS

- PRINCIPAL INVESTIGATOR of *POLYPHEMO PROJECT* (390.000 EURO) granted through competitive call IIT-SEED 2009
- CNR Unit Progetto *M2M NETERGIT* (600.000 EURO) granted through EU PON
- INVITED TOPICAL REVIEW on Modeling hybrid perovskites by molecular dynamics
- several HIGHLY CITED PAPERS according to ISI during years 2015-2020

**RESEARCH
DESCRIPTION**

The activity is focused on the development and use of **theoretical-computational methods** for the study and design at the nanoscale of materials for energy, opto- and nano- electronics based on organic-inorganic and order/disorder hybrid systems. Distinguishing feature of the research is to include the **effects of thermodynamics and structural complexity** of materials. Results of the research activity concerns the microstructure evolution (point- or extended defects, recrystallization and phase transformation, self-assembling phenomena) and the study of **thermodynamic and optoelectronic properties of hybrid nanomaterials** in realistic conditions.

**RECENT
ADVANCEMENTS**

Most relevant recent advancements concern polymer/oxide systems and hybrid perovskites. In particular, the first interatomic potential for **classical molecular dynamics** of *hybrid perovskites* (Mattoni et al., JPCC 2015, 119,17421) is particularly original result in the field of one of the most important innovative materials for photovoltaics.

IMPACT

The above methodology has made affordable the study crucial aspects of the material related to defects diffusion, molecular rotational disorder, thermal transport, vibrational properties, electro-caloric effects, degradation in presence of water. In 2017, four publications have been classified by ISI WoS as **"highly cited papers"** (placed in the top 1% of the academic field of Chemistry based on a highly cited threshold for the field and publication year).

A.M. has published an **invited "topical review"** in Journal Physics:Condensed Matter (2017) on molecular dynamics simulations of hybrid perovskites

**INTERNATIONAL
RELEVANCE**

High impact publications and several continuative collaborations with research centers at the forefront of materials science. (CNRS-Marseille, France; CSM Colorado, USA; Graetzel group@EPFL, Lausanne, CH; Yamashita's research lab, University of Tokyo, JAP). Model potentials for hybrid perovskites have a considerable international impact (30 citations / year and several tens of international collaborations)

FUND RAISING

> 1Meuro since 2010, by competitive calls for scientific proposals.

A.M. has been granted by a national project from Italian Institute of Technology (IIT-SEED POLYPHEMO).

SCIENTIFIC PRODUCTION

Bibliometric indicators
(update June 2020)

BIBLIOMETRIC DESCRIPTORS (JUNE 2020)	SOURCE	NUMBER OF PUBLICATIONS	CITATIONS	H INDEX
	GOOGLE SCHOLAR	120	2870	31
	SCOPUS	98	2265	27
	WOS	95	2145	26

EDUCATION

- 21/02/2003 PhD in Physics
University of **Padova** (PD)
- 23/07/1998 Master Degree in Physics (110 e Lode)
University of **Perugia** (PG)
- 1991 High School (60/60)
Liceo Scientifico G. Marconi, **Foligno** (PG)

PROFESSIONAL EXPERIENCE

- 01-02-2010 to 14-10-2020 Staff Researcher
CNR-IOM Cagliari, National Council of Research
- 2008-2010 Tenure Track Researcher T.D.
CNR-INFN, National Council of Research, **Cagliari**
- 2005-2008 Researcher T.D. - European Project FP6 NANOPHOTO
National Institute of Physics of Matter, Regional Laboratory "Sardinian Laboratory for Computational Materials Science", **Cagliari**
- 2005-2005 Research Contract
High Performance Computing Center, CASPUR, **Roma**, Italia
- 2004-2004 Research Contract
Department of Physics, University of **Cagliari**, Monserrato (CA), Italia
- 2002-2004 Post-doc
National Institute of Physics of Matter, Unit of **Cagliari**, Monserrato (CA), Italia
- 2000-2002 PhD Grant
Department of Physics, University of **Padova**
- 1998-1999 Research Collaborator

Department of Physics, University of Perugia

Habitations

- 2020 Eligible as "CNR- Director of Research"
CNR call 367.160 (2017)
- 2020,2012 Italian Scientific University Teaching Habilitation (ANVUR ASN FIS02/B2)
Associated Professor (IIa fascia)
- 2008 French National Scientific University Teaching Habilitation
"Qualification aux fonctions de maître de conférences"

FUNDING BY
COMPETITIVE GRANTS
(2010-2016) >1 Millions Euro

LIST OF PROJECTS

REGIONAL PROJECTS

NATIONAL PROJECTS

<i>FUNDING AGENCY</i>	<i>AMOUNT (Euro)</i>	<i>Period</i>	<i>role of A. Mattoni</i>	<i>Project Title</i>
Autonomous Region of Sardinia	50.000	2010-2014	Unit Coordinator	CdS/Pt Photocatalysts for water splitting by solar energy
Autonomous Region of Sardinia	56.000	2011-2015	Unit Coordinator	Design of hybrid eco-friendly nanomaterials for photovoltaics
National Council of Research	10.000		Unit Coordinator IOM Cagliari	National Project on organic photovoltaics (OPV) of the "Rete Nazionale" del CNR
CompuNet Italian Institute of Technology	~ 60.000 two years senior post-doc contract	2013-2015	Unit Coordinator	Multi scale modeling of hybrid nanomaterials for energy and optoelectronic
Foundation "Banco di Sardegna"	13.000	2015	Coordinator	Modeling nanohybrids

EUROPEAN PROJECTS

EU through Programma Operativo Nazionale 2007-2013 "Ricerca e competitività	600.000 (total cost 5Meuro)	2017-2019	Coordinator Unit CNR	Network for Energy and Internet of Things Ricerca Applicata a Reti di comunicazione M2M e modem integrati innovativi dedicati a servizi avanzati per le Smart Cities
~ 10 progetti ISCRA C	> 2 Millions cpu hours;	2010-2017	Principal Investigator	TIPTAP, PICO THESTA, OPTOBIS SOAP, SWING SPASS, THEHYPER, VIPER, MYPALLOY
ISCRA B	3 Millions cpu hours	2017-2018	Principal Investigator	UNWRAPIT
Italian Institute of Technology	390.000 (granted through national competitivit e call IIT-SEED 2009)	2010-2013	Principal investigator and Coordinator	POLYmer based hYbrid nanomaterials for PHotovoltaics: improving Efficiency by theoretical MOdeling
PRACE 14th CALL "Partnership for Advanced Computing in Europe	54 Millions CPU hours	2017-2018	Principal Investigator and Coordinator	UNWRAP UNderstanding Water induced degRAdation of hybrid Perovskites
PRACE 17th CALL "Partnership for Advanced Computing in Europe	33 Millions CPU HOURS	2018-2019	Principal Investigator and Coordinator	DECONVOLVES Determining watEr COntact aNgle on eVOLving peroVskitEs Surfaces
EU FP6		2005-2008	Coordinator modeling tasks at	NANOPHOTO: Nanocrystalline thin films for low

			SLACS- INFN Cagliari	cost photovoltaics and optoelectronics
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DIRECTION OF RESEARCH GROUPS

- 2018-present Person in charge of the Unit of Cagliari of Institute of Matter CNR-IOM Cagliari
CNR-IOM Cagliari
- 2010-2015 Coordinator of Project MD.P06.14 (commessa CNR IOM-Cagliari)
Teoria e modeling di materiali e processi per le nanoscienze
- 2010-2020 Coordinator Group Hybrid Nanomaterials for Energy and Optoelectronics (Mattoni
Research Group www.dsf.uica.it/~mattoni)
Mattoni Research Group (www.dsf.uica.it/~mattoni)

PANELS/COMMITTEE

- 2019-2020 Steering Committee, Graduate Course in Electric and Electronic Engineering
Department of Electric and Electronic engineering, University of Cagliari
- 2018 Steering Committee, Graduate Course in Physics
Department of Physics, University of Cagliari
- 2017 PhD Evaluation Panel
Università di Bologna
- 2017 PhD Evaluation Panel
Scuola di Dottorato del Politecnico di Torino
- 2014-2014 PhD Evaluation Panel
University of Atlantico, U de C del Doctorado en Ciencias Físicas - SUE Caribe
(Colombia)
- 2010-2016 Expert Reviewer CINECA
ISCR supercomputing initiative
- 2015-2016 Panel of European Material Modeling Council
European Material Modeling Council
- 2010-2015 Panel "Computational Platform" CompuNet-IIT
Istituto Italiano di Tecnologia

- 2010-2015 Examination Board for CNR post-doc and research selections
> 10 including Researcher, post-doc junior e senior
- 2010-2015 Evaluation Board for post-doc selections Università degli Studi di Cagliari
1 post-doc

CONFERENCES ORGANIZATION

- 2012 (Local organizer and board member) CECAM Workshop, Energy from the Sun: Theoretical Physicists and Chemists take up the Challenge
Chia Laguna, Cagliari, Italy
- 2011 (organizing committee) DMD-TeoC
CNR, Rome, Italy
- 2007 (Local organizer) FP6 NANOPHOTO Workshop
University of Cagliari, Italy

SELECTION OF INVITED TALKS

- 2020 *Keynote speaker*
"Structure and dynamics of halide perovskites";
nanoGe Internet Conference titled "Theory and Computation of Halide Perovskites (ComPer)"
- 2020 "Ionic dynamics in nanostructured hybrid perovskites: insights from classical molecular dynamics";
iNANO 2020, Webinar on Nanotechnology, ScifedonLine (online conference)
- 2016 "Understanding thermally activated phenomena in hybrid organic-inorganic halide perovskites by molecular dynamics simulations" Invited Talk
Dipartimento di Ingegneria Civile e Ambientale, Università di Perugia
- 2015 "The role of atomistic simulations in the research on hybrid photovoltaics"
Nanoltaly 2015, Chiostro rinascimentale del Sangallo, Sapienza Università di Roma, Italy
- 2015 "Atomistic investigation of hybrid perovskites for photovoltaics",
International Workshop on Applied Materials for Science and Technology- University of Atlantico, Cartagena, Colombia
- 2015 "Dynamical properties of hybrid perovskites by large scale model potential

molecular dynamics”

CECAM Workshop “Theoretical modeling and simulation of perovskite-based solar cells” Lausanne, CH

2014 “Modeling hybrid nanomaterials for photovoltaics”

Renewable Energy Materials Research Science and Engineering Center, CO, USA

2013 “Self-assembled interlayers at the polymer/metaloxide interface: electronic properties and morphology”

Center for Hybrid and Organic Solar Energy and Department of Electronic Engineering, Università Roma “Tor Vergata”

2012 “Model potential molecular dynamics simulations of nanostructured materials for photovoltaics”

International Center for Theoretical Physics, Miramare

2010 “Modeling at the atomic scale the morphology of polymer based hybrids for photovoltaics”

Centre Interdisciplinaire de Nanoscience de Marseille, CNRS-CINaM, Marseille, France

TEACHING ACTIVITY

2019-2021 "An introduction to the atomistic simulations of hybrid materials" course for PhD in Physics

PhD in Physics, Department of Physics, University of Cagliari

2018-2019 "Introduzione alla simulazione atomistica dei materiali ibridi" corso di laurea in Fisica - Percorso di Eccellenza"

Department of Physics, University of Cagliari

2015 “Theoretical Modelling and simulation of perovskite-based solar cells”

CECAM workshop, Switzerland, CH

2015 Course for PhD Students “Introduction to computational materials physics”

Scuola Superiore di Catania, Università degli Studi di Catania, Catania, Italy

2012 Course at the international school "Introduction to classical MD, models of interaction, simulation of nanostructured materials, interfaces

"School on Numerical Methods for Materials Science Related to Renewable Energy Applications" - International Centre for Theoretical Physics, ICTP, Trieste TS, Italy

2008-2009 Post-lauream master course “ Atomistic simulations & Nanoprobing ”

Interuniversity Master in Nanotechnology, CIVEN, Mestre (VE), Italy

2007 post-lauream master course “Principle of photoconversion”

Sardegna Ricerche - International Master on Renewable Energy, Monteponi, Iglesias, Italy

SCIENTIFIC SUPERVISION

- 2010-2020 4 post-doc researchers (~16 year- person)
CNR
- 2010-2015 3 post-doc researchers (~4 person years)
Dipartimento di Fisica, Università degli Studi di Cagliari
- 2013-2015 1 post-doc contract
CompuNet, Istituto Italiano di Tecnologia
- 2003-2006 1 post-doc
INFM SLACS Cagliari
- 2003-2006 co-supervisor 1 PhD
Dipartimento di Fisica, Universitat Autònoma de Barcelona, ICMAB-CSIC, SPAIN
- 2016 co-supervisor 1 PhD
Department of Chemical System Engineering, University of Tokyo, JAPAN
- 2008-2011 co-supervisor 1 PhD
Dipartimento di Ingegneria Energetica, Università di Roma La Sapienza
- 2006-2015 co-supervisor 4 PhD
Dipartimento di Fisica, Università degli Studi di Cagliari
- 2003-2013 4 Degree Students
Dipartimento di Fisica, Università degli Studi di Cagliari
- 2003-2013 2 Degree Students
Dipartimento di Ingegneria Elettrica ed Elettronica, Università degli Studi di Cagliari

REVIEWING ACTIVITY

JOURNALS

Reviewing activity of several high IF journals including:

- ACS (JPCC, JPCL, ACS Nano, Nanoletters)
- APS (Phys Rev B, Phys, Rev)
- Nature Publishing Group (Nature Comm., Nature Materials, Scientific Reports)
- RCS (Nanoscale, Phys Chem Chem Phys, Energy)
- Elsevier (Nanoenergy, Solar Energy)
- Institute of Physics (J. of Physics, Condensed Matter)

NATIONAL AND INTERNATIONAL GRANTING

Reviewer for granting support of Dutch Research Council (NWO) domain Applied and Engineering Sciences (AES)

Reviewer for ISCRA for HPC resources within ISCRA Initiative

SELECTION OF PUBLICATIONS

Year	Title	Journal	IF	citations/year (scopus)
2011	The effect of... https://doi.org/10.1039/C2EE22212D	Energy Env. Sci.	32.15	4
2017	Toward High-Temperature Stability... https://doi.org/10.1002/aenm.201601486	Adv. Energy Mater.	24.88	7
2014	Interfacial engineering of ... https://doi.org/10.1002/aenm.201301694	Adv. Energy Mater.	24.88	4
2014	Colloidal Bi ₂ S ₃ nanocrystals: https://doi.org/10.1002/adfm.201303879	Adv. Func. Mater.	15.6	7
2016	Origin of unusual... https://doi.org/10.1126/sciadv.1601156	Science Advances	12.53	29
2017	Collective Molecular Mechanisms... https://doi.org/10.1021/acsnano.7b04116	ACS Nano	13.7	4
2017	Self-Assembled Lead Halide... https://doi.org/10.1021/acsenergylett.7b00046	ACS Energy Lett.	14.6	2
2020	The dominant role... https://doi.org/10.1016/j.nanoen.2019.104162	NanoEnergy	15.2	1
2015	Competing forces in... https://doi.org/10.1021/acsnano.5b00809	ACS Nano	13.7	2
2019	Dual effect of... https://doi.org/10.1039/C9TA00715F	J. Mater. Chem. A	10.42	5
2005	Atomic scale origin... https://doi.org/10.1103/PhysRevLett.95.115501	Phys. Rev. Lett.	9.2	5
2016	Thermally Activated Point... https://doi.org/10.1021/acs.jpcclett.6b00963	J. Phys. Chem. Lett.	7.3	12
2016	Temperature Evolution of .. https://doi.org/10.1021/acs.jpcclett.5b02546	J. Phys. Chem. Lett.	7.3	10
2015	Methylammonium Rotational... https://doi.org/10.1021/acs.jpcc.5b04283	J. Phys. Chem.	4.3	24
2014	Radiative recombination and... https://doi.org/10.1021/jp507430x	J. Phys. Chem.	4.3	9
2014	Hybrid perovskites for... https://doi.org/10.1103/PhysRevB.89.125203	Phys. Rev. B	3.72	19

List of Publications
(only 2014-2020 are
reported)
the full list of publications
at google scholar

<https://scholar.google.it/citations?user=Y1hzoDAAAAAJ&hl=en>

Ion Migration - Induced Amorphization and Phase Segregation as a Degradation Mechanism in Planar Perovskite Solar Cells

D Di Girolamo, N Phung, FU Kosasih, F Di Giacomo, F Matteocci, ...
Advanced Energy Materials, 2000310

2020

Direct correlation of nanoscale morphology and device performance to study photocurrent generation in donor enriched phases of polymer solar cells

S Ben Dkhil, P Perkhun, C Luo, D Müller, R Alkarsifi, E Barulina, ...
ACS Applied Materials & Interfaces

2020

The Role of Grain Boundaries on Ionic Defect Migration in Metal Halide Perovskites

N Phung, A Al - Ashouri, S Meloni, A Mattoni, S Albrecht, EL Unger, ...
Advanced Energy Materials, 1903735

2020

Ultralow thermal conductivity of two-dimensional metal halide perovskites

A Giri, AZ Chen, A Mattoni, K Aryana, D Zhang, X Hu, SH Lee, JJ Choi, ...
Nano Letters

2020

Dielectric function of hybrid perovskites at finite temperature investigated by classical molecular dynamics

A Mattoni, C Caddeo
The Journal of Chemical Physics 152 (10), 104705

2020

Ag/In lead - free double perovskites

F Liu, D Marongiu, R Pau, V Sarritzu, Q Wang, S Lai, AG Lehmann, ...
EcoMat 2 (1), e12017

2020

The dominant role of surfaces in the hysteretic behavior of hybrid perovskites

C Caddeo, A Filippetti, A Mattoni
Nano Energy, 104162

2019

Donuts and Spin Vortices at the Fermi Surfaces of Hybrid Lead-Iodide CH₃NH₃PbI₃ Perovskites

A Filippetti, C Caddeo, A Bosin, P Delugas, A Mattoni
The Journal of Physical Chemistry C 123 (11), 6753-6762 2019

2019*Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide*

C Caddeo, D Marongiu, S Meloni, A Filippetti, F Quochi, M Saba, ...

Advanced Materials Interfaces 6 (3), 1801173 2

2019*Layered Germanium Hybrid Perovskite Bromides: Insights from Experiments and First-Principles Calculations*

X Chang, D Marongiu, V Sarritzu, N Sestu, Q Wang, S Lai, A Mattoni, ...

Advanced Functional Materials, 1903528

2019*Dual effect of humidity on cesium lead bromide: enhancement and degradation of perovskite films*

D Di Girolamo, MI Dar, D Dini, L Gontrani, R Caminiti, A Mattoni, ...

Journal of Materials Chemistry A 7 (19), 12292-12302 3

2019*Machine Learning-Based Charge Transport Computation for Pentacene*

J Lederer, W Kaiser, A Mattoni, A Gagliardi

Advanced Theory and Simulations, 1800136 2

2018*Linking morphology to thermal conductivity in PEDOT: an atomistic investigation*

C Genovese, A Antidormi, R Dettori, C Caddeo, A Mattoni, L Colombo, ...

Journal of Physics D: Applied Physics 50 (49), 494002 1

2017*Collective Molecular Mechanisms in the CH₃NH₃PbI₃ Dissolution by Liquid Water*

C Caddeo, MI Saba, S Meloni, A Filippetti, A Mattoni

ACS nano 11 (9), 9183-9190

2017*Bulk Structural and Electronic Properties at the Density Functional Theory and Post-Density Functional Theory Level of Calculation*

MH Du, A Filippetti, A Mattoni, C Caddeo

Theoretical Modeling of Organohalide Perovskites for Photovoltaic ...

2017■ *Structure and Thermodynamic Properties of Hybrid Perovskites by Classical Molecular Dynamics*

C Caddeo, A Filippetti, A Mattoni

Theoretical Modeling of Organohalide Perovskites for Photovoltaic ...

2017■ *Bulk Structural and Electronic Properties at the Density Functional Theory and Post-Density Functional Theory Level of Calculation*

C Caddeo, A Mattoni, A Filippetti, MH Du

Theoretical Modeling of Organohalide Perovskites for Photovoltaic ...

2017

Self-assembled lead halide perovskite nanocrystals in a perovskite matrix

D Marongiu, X Chang, V Sarritzu, N Sestu, R Pau, A Geddo Lehmann, ...
ACS Energy Letters 2 (4), 769-775 5

2017

Confinement of vibrational modes within crystalline lattices using thin amorphous layers

L Bagolini, A Mattoni, MT Lusk

Journal of Physics: Condensed Matter 29 (14), 145302

2017

Development of a classical interatomic potential for MAPbBr₃

T Hata, G Giorgi, K Yamashita, C Caddeo, A Mattoni

The Journal of Physical Chemistry C 121 (7), 3724-3733 2

2017

Toward high - temperature stability of PTB7 - based bulk heterojunction solar cells: impact of fullerene size and solvent additive

SB Dkhil, M Pfannmöller, MI Saba, M Gaceur, H Heidari, ...

Advanced Energy Materials 7 (4) 17

2017

Photoluminescence, optical gain, and lasing threshold in CH₃NH₃PbI₃ methylammonium lead-halide perovskites obtained by ab initio calculations

A Filippetti, C Caddeo, P Delugas, A Mattoni

Journal of Materials Chemistry C 5 (48), 12758-12768

2017

Appealing Perspectives of hybrid lead-iodide perovskites as thermoelectric materials

A Filippetti, C Caddeo, P Delugas, A Mattoni

The Journal of Physical Chemistry C 120 (50), 28472-28479 7

2016

Modeling hybrid perovskites by molecular dynamics

A Mattoni, A Filippetti, C Caddeo

Journal of Physics: Condensed Matter 29 (4), 043001 12

2016

Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites

MI Dar, G Jacopin, S Meloni, A Mattoni, N Arora, A Boziki, ...

Science advances 2 (10), e1601156 49

2016

Surface Polarization Drives Photoinduced Charge Separation at the P3HT/Water Interface

E Mosconi, P Salvatori, MI Saba, A Mattoni, S Bellani, F Bruni, ...

ACS Energy Letters 1 (2), 454-463 17

2016

Thermally activated point defect diffusion in methylammonium lead trihalide: anisotropic and ultrahigh mobility of iodine

P Delugas, C Caddeo, A Filippetti, A Mattoni

The journal of physical chemistry letters 7 (13), 2356-2361 31

2016

Temperature evolution of methylammonium trihalide vibrations at the atomic scale

A Mattoni, A Filippetti, MI Saba, C Caddeo, P Delugas
The Journal of Physical Chemistry Letters 7 (3), 529-535 36

2016

Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure

C Caddeo, C Melis, MI Saba, A Filippetti, L Colombo, A Mattoni
Physical Chemistry Chemical Physics 18 (35), 24318-24324 15

2016

Low electron-polar optical phonon scattering as a fundamental aspect of carrier mobility in methylammonium lead halide $CH_3NH_3PbI_3$ perovskites

A Filippetti, A Mattoni, C Caddeo, MI Saba, P Delugas
Physical Chemistry Chemical Physics 18 (22), 15352-15362 26

2016

Entropy-suppressed ferroelectricity in hybrid lead-iodide perovskites

A Filippetti, P Delugas, MI Saba, A Mattoni
The Journal of Physical Chemistry Letters 6 (24), 4909-4915 29

2015

Pinpointing the Cause of Platinum Tipping on CdS Nanorods

C Caddeo, V Calzia, L Bagolini, MT Lusk, A Mattoni
The Journal of Physical Chemistry C 119 (39), 22663-22668 5

2015

Methylammonium rotational dynamics in lead halide perovskite by classical molecular dynamics: the role of temperature

A Mattoni, A Filippetti, MI Saba, P Delugas
The Journal of Physical Chemistry C 119 (30), 17421-17428 93

2015

Atomistic Modeling of Morphology and Electronic Properties of Colloidal Ultrathin Bi_2S_3 Nanowires

V Calzia, R Piras, A Ardu, A Musinu, M Saba, G Bongiovanni, A Mattoni
The Journal of Physical Chemistry C 119 (29), 16913-16919 6

2015

Methylammonium fragmentation in amines as source of localized trap levels and the healing role of Cl in hybrid lead-iodide perovskites

P Delugas, A Filippetti, A Mattoni
Physical Review B 92 (4), 045301 33

2015

Intrinsic origin of two-dimensional electron gas at the (001) surface of $SrTiO_3$

P Delugas, V Fiorentini, A Mattoni, A Filippetti
Physical Review B 91 (11), 115315 10

2015

Competing forces in the self-assembly of coupled ZnO nanopillars
E Javon, M Gaceur, W Dachraoui, O Margeat, J Ackermann, MI Saba, ...

ACS nano 9 (4), 3685-3694 15

2015

The study of polythiophene/water interfaces by sum-frequency generation spectroscopy and molecular dynamics simulations

S Bellani, M Porro, C Caddeo, MI Saba, PB Miranda, A Mattoni, G Lanzani, ...

Journal of Materials Chemistry B 3 (31), 6429-6438 6

2015

Radiative recombination and photoconversion of methylammonium lead iodide perovskite by first principles: properties of an inorganic semiconductor within a hybri...

A Filippetti, P Delugas, A Mattoni

The Journal of Physical Chemistry C 118 (43), 24843-24853 43

2014

Atomistic Simulations of P (NDI2OD-T2) Morphologies: From Single Chain to Condensed Phases

C Caddeo, D Fazzi, M Caironi, A Mattoni

The Journal of Physical Chemistry B 118 (43), 12556-12565 10

2014

Interfacial engineering of P3HT/ZnO hybrid solar cells using phthalocyanines: a joint theoretical and experimental investigation

G Mattioli, SB Dkhil, MI Saba, G Mallocci, C Melis, P Alippi, F Filippone, ...

Advanced Energy Materials 4 (12) 17

2014

Effects of TIPS-functionalization and perhalogenation on the electronic, optical, and transport properties of angular and compact dibenzochrysene

R Cardia, G Mallocci, A Mattoni, G Cappellini

The Journal of Physical Chemistry A 118 (28), 5170-5177 19

2014

Carrier Localization in Nanocrystalline Silicon

L Bagolini, A Mattoni, RT Collins, MT Lusk

The Journal of Physical Chemistry C 118 (25), 13417-13423 9

2014

Atomistic simulations of thiol-terminated modifiers for hybrid photovoltaic interfaces

G Mallocci, A Petrozza, A Mattoni

Thin Solid Films 560, 34-38

2014

Colloidal Bi2S3 nanocrystals: quantum size effects and midgap states

M Aresti, M Saba, R Piras, D Marongiu, G Mula, F Quochi, A Mura, ...

Advanced Functional Materials 24 (22), 3341-3350 44

2014

Hybrid perovskites for photovoltaics: Insights from first principles

A Filippetti, A Mattoni

Physical Review B 89 (12), 125203 108

2014

Effect of thermodynamics and curvature on the crystallinity of P3HT thin films on ZnO: insights from atomistic simulations

MI Saba, A Mattoni

The Journal of Physical Chemistry C 118 (9), 4687-4694 9

2014

Thermally induced recrystallization of textured hydrogenated nanocrystalline silicon

G Fugallo, A Mattoni

Physical Review B 89 (4), 045301 14

2014

Angular and Compact Dibenzochrysene: the Role of Functionalizations on their Electronic and Optical Properties

R Cardia, G Cappellini, A Mattoni

European Theoretical Spectroscopy Facility Young Researchers' Meeting
2014

2014

Simulations of oxide/polymer hybrids

MI Saba, A Mattoni

Encyclopedia of Nanotechnology, 1-13 3

2014

Colloidal synthesis and characterization of Bi₂S₃ nanoparticles for photovoltaic applications

R Piras, M Aresti, M Saba, D Marongiu, G Mula, F Quochi, A Mura, ...

Journal of Physics: Conference Series 566 (1), 012017 4

2014

Cagliari, 8 novembre 2020

Alessandro Mattoni

