CURRICULUM VITAE

EDOARDO MOSCONI

Personal Data:

Date and place of birth: 1982,

Citizenship:

Spoken Languages: **Italian (mother tongue), English (fluent written and oral).**

Bibliometric Information and Scientific Production

Source: Google Scholar, https://scholar.google.it/citations?user=frrxchwAAAAJ&hl=it (02/01/2024)

H-index	**65**
Citations	**27548**
i10-index	**120**
Publications	**142 ISI Journals**
Book chapters	**4**
Most Cited Article	**2072 citations: https://doi.org/10.1002/aenm.201500477**
Reviewer Activity	Reviewer for the following journals: Chemistry of Materials, ACS Applied Materials & Interfaces, Journal of Materials Chemistry A, Journal of Physical Chemistry, ACS Energy Letters.

Current Position

01/01/2023 – **Senior Research Scientist at CNR-SCITEC, Perugia, Italy**. Computational Laboratory for Hybrid/Organic Photovoltaics - www.clhyo.org/people-left/7-edoardo-mosconi.html

Previous Positions

15/09/2017 to 31/12/2022 - **Research Scientist at CNR-SCITEC, Perugia, Italy**. Computational Laboratory for Hybrid/Organic Photovoltaics - www.clhyo.org/people-left/7-edoardo-mosconi.html
February 2015 – September 2017: **Senior Post Doctoral Researcher of Italian Institute of Technology (IIT), Genoa, Italy.**
January 2012 – February 2015: **Post-Doctoral Researcher at CNR-ISTM, Perugia, Italy.**
September 2010 – December 2010: **Visiting Scientist, Department of Chemistry, Princeton University, USA.**

Education

November 2008 – November 2011: **PhD in Chemistry,** University of Perugia and CNR-ISTM, Perugia, Italy. **PhD Degree date: 24 November 2011**.
PhD Thesis: "*Computational Modeling of Hybrid/Organic Photovoltaics and Complex Reaction Mechanisms.*" Advisors: Dr. Filippo De Angelis (CNR-ISTM, Perugia, Italy), Prof. Antonio Sgamellotti (University of Perugia, Italy).
November 2007 – October 2008: **Post-graduate scholarship**, University of Perugia, Italy.
26 October 2007: **Master degree in Organic Chemistry** at the University of Perugia, Italy (110/110 cum laude)
Thesis: "*Theoretical Investigation of base-catalyzed β-elimination Reactions in Water Solution for Systems Activated by the Pyridine Ring.*" Advisors: Prof. S. Alunni (University of Perugia, Italy), Dr. Filippo De Angelis (CNR-ISTM, Perugia, Italy) and Prof. F. Tarantelli (University of Perugia, Italy).
April 2004: **Bachelor degree in Chemistry** at the University of Perugia, Italy (110/110 cum laude).
Thesis: "*Sistemi anfifilici nanostrutturati*". Advisors: Prof. G. Savelli (University of Perugia, Italy) and Prof. R. Germani (University of Perugia, Italy)

Schools

January 2008: **WiS-POC 2008**, Bressanone
September 2009: **PCAM summer School**, Milano Bicocca University

Track Record

I have authored more than 140 papers and 4 book chapters in the field of new generation photovoltaic materials reaching an h-index of 65 and a total of more than 27000 citations (source Google Scholar, 02/01/2024). I am also in the ***"highly cited researcher"*** list from 2018 to 2023 underlining the important impact and influence of my research activity in the field of photovoltaics and more in general in the global science community. I have pioneered the field of theoretical/computational modeling of organohalide perovskites for solar cells applications. I authored the first paper on the

subject (*J. Phys. Chem. C* **2013**, *117*, 13902-13913), which was the most read article in J. Phys. Chem. C published in 2013, despite it was published in June, as from the announcement made by J. Phys. Chem. C in April 2014. This article has gathered 947 citations (source Google Scholar, 17/02/2022). After this initial study, I developed an effective GW method incorporating spin-orbit coupling which allows to accurately model the electronic, optical and transport properties of halide perovskites (*Sci. Rep.* **2014**, 4, 4467). In particular, the implementation of this innovative and more efficient computational approach of GW in Quantum Espresso program package opens the way to the extensive and fundamental understanding of the peculiar and impressive properties of this class of materials. This paper, published in 2014, is now the reference work representing the state-of-art approach for the computational simulation of this materials obtaining 1154 citations (source Google Scholar, 17/02/2022).

I have continued to investigate the electronic and optical properties of organohalide perovskites in a series of several subsequent papers devoted to perovskite solar cells modeling. The developments he has contributed deal with the broadest possible description of these materials, including their structural, electronic, spectroscopic and interfacial properties. A list of my main achievements is reported below:

- I co-authored the first theoretical simulations of the Raman and IR spectra of methylammonium lead iodide, allowing the assignment of the respective experimental spectra (*J. Phys. Chem. Lett.* **2014**, 5, 279 and *Phys. Chem. Chem. Phys.* **2014**, 16, 16137).
- I co-authored the first theoretical simulation of chloride doping into methylammonium lead iodide, allowing the interpretation of experimental XRD data (*Chem. Mater.* **2013**, 25, 4613).
- I co-authored the first study reporting relativistic GW calculations on methylammonium lead iodide and methylammonium tin iodide, allowing for the first time to obtain an adequate and accurate description of the electronic properties of this class of materials. (*Sci. Rep.* **2014**, 4, 4467).
- I have authored the first study highlighting the interplay of structural and spin-orbit electronic features in determining band-gap tuning in organohalide led perovskites (*Nano Lett.* **2014**, 14, 3608).
- I have authored and co-authored the first studies on the interface between methylammonium lead iodide and TiO_2 semiconductor (*J. Phys. Chem. Lett.* **2014**, 5, 2619, *Nano Lett.* **2014**, 14, 2168, *J. Phys. Chem. Lett.* **2014**, 5, 3532).
- I have authored of the first study on the perovskite degradation process operated by water (*Chem. Mater.* **2015**, 27, 4885-4892).
- I have authored of the first study focused on the role of defects at the perovskite/TiO_2 interface (*Energy Environ. Sci.* **2015**, 8, 2118-2127).

• I have published the first study on the role of light in promoting the annihilation of Frenkel defects in organohalide perovskites (*Energy Environ. Sci.* **2016**, 9, 3180-3187).

• I contributed to the study of the interface engineering focused on increasing the device stability (*Nat Commun* **2017**, 8, 15684).

• I contributed to study and develop an alternative HTM for low-cost and efficient device fabrication (*Nat. Energy* **2016**, *1*, 15017).

• I carried out the first study in understanding the role of defect in determining the structural response of the perovskite materials under electric field exposure (*Nat. Mater.* **2018**, 17, 1020-1026).

• I contributed to increase the stability of perovskite devices using surface passivation approach (*Science*, **2019**, 365, 473–478).

• I contributed to understand how to achieve bandgap stability by a ligand engineering approach (*Nature*, **2021**, 591, 72–77).

In summary, I have launched and now I am leading the field of perovskite solar cells modeling.
I had also carried out several publications on the field of Dye Sensitized Solar Cells (DSSCs), Organic Photovoltaics (OPV) and quantum-dot materials, giving an important contribution to the understanding of the electronic and optical properties of the employed components and the devices working mechanisms.

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Mosconi, E.; Yum, J. H.; Kessler, F.; Gomez-Garcia, C. J.; Zuccaccia, C.; Cinti, A.; Nazeeruddin, M. K.; Graetzel, M.; De Angelis, F. "Cobalt Electrolyte/Dye Interactions in Dye-Sensitized Solar Cells: A combined Computational and Experimental Study" *J. Am. Chem. Soc.* **2012**, *134*, 19438.	**14.36**	**244**	**First Author**
Mosconi, E.; Amat, A.; Nazeeruddin, M. K.; Graetzel, M.; De Angelis, F. "First Principles Modeling of Mixed Halide Organometal Perovskites for Photovoltaic Applications" *J. Phys. Chem. C* **2013**, 117, 13902.	**4.69**	**1057**	**First Author**
Umari, P.; **Mosconi, E.**; De Angelis, F. "Relativistic GW calculations on $CH_3NH_3PbI_3$ and $CH_3NH_3SnI_3$ Perovskites for Solar Cell Applications" *Sci. Rep.* **2014**, *4*, 4467.	**4.12**	**1363**	**Author**
Azpiroz, J. M.; **Mosconi, E.***; Bisquert, J.; De Angelis, F. "Defects Migration in Methylammonium Lead Iodide and their Role in Perovskite Solar Cells Operation" *Energy Environ. Sci.* **2015**, *8*, 2118.	**30.07**	**1490**	**Corresponding Author**
Amat, A.; **Mosconi, E.***; Ronca, E.; Quarti, C.; Umari, P.; Nazeeruddin, M. K.; Grätzel, M.; De Angelis, F. "Cation-Induced Band-Gap Tuning in Organohalide Perovskites: Interplay of Spin–Orbit Coupling and Octahedra Tilting" *Nano Lett.* **2014**, *14*, 3608.	**12.08**	**1210**	**Corresponding Author**

Mosconi, E.*; Meggiolaro, D.; Snaith, H. J.; Stranks, S. D.; De Angelis, F. "Light-induced annihilation of Frenkel defects in organo-lead halide perovskites" *Energy Environ. Sci.* **2016**, *9*, 3180.	**30.07**	**348**	**First and Corresponding Author**
Mosconi, E.*; Azpiroz, J. M.; De Angelis, F. "Ab Initio Molecular Dynamics Simulations of Methylammonium Lead Iodide Perovskite Degradation by Water" *Chem. Mater.* **2015**, *27*, 4885.	**9.89**	**467**	**First and Corresponding Author**
Mosconi, E.*; Umari, P.; De Angelis, F. "Electronic and Optical Properties of Mixed Sn-Pb Organohalide Perovskites: a First Principles Investigation" *J. Mater. Chem. A* **2015**, *3*, 9208.	**9.93**	**192**	**First and Corresponding Author**
Saliba, M.; Orlandi, S.; Matsui, T.; Aghazada, S.; Cavazzini, M.; Correa-Baena, J.-P.; Gao, P.; Scopelliti, R.; **Mosconi, E.**; Dahmen, K.-H. "A molecularly engineered hole-transporting material for efficient perovskite solar cells" *Nat. Energy* **2016**, *1*, 15017.	**46.86**	**926**	**Author**
Chen, B.; Li, T.; Dong, Q.; **Mosconi, E.**; Song, J.; Chen, Z.; Deng, Y.; Liu, Y.; Ducharme, S.; Gruverman, A.; Angelis, F. D.; Huang, J. "Large electrostrictive response in lead halide perovskites" *Nat. Mater.* **2018**, *17*, 1020.	**47.53**	**149**	**Author**

Research activities

First Principles Modeling organohalide lead perovskites for photovoltaics applications

Hybrid AMX_3 perovskites (A=Cs, CH_3NH_3; M=Sn, Pb; X=halide) have in the last years revolutionized the scenario of emerging photovoltaic technologies.

The $CH_3NH_3PbI_3$/$MAPbI_{3-x}Cl_x$ perovskites have dominated the field, while the similar $CH_3NH_3SnI_3$ has been less explored for photovoltaic applications. Replacement of Pb by Sn would facilitate the large uptake of perovskite-based photovoltaics.

Despite the extremely fast progress, the materials electronic properties which are key to the photovoltaic performance are relatively little understood.

Density Functional Theory electronic structure methods have so far delivered an unbalanced description of Pb- and Sn-based perovskites. I contributed to develop an effective GW method incorporating spin-orbit coupling which allows us to accurately model the electronic, optical and transport properties of halide perovskites, opening the way to new materials design. In particular the different $CH_3NH_3SnI_3$ and $CH_3NH_3PbI_3$ electronic properties are discussed in light of their exploitation for solar cells, and found to be dominantly due to relativistic effects.

By applying our computational approach, I moved to investigate the effect of the chlorine doping for the mixed halide perovskites ($MAPbI_{3-x}Cl_x$), the role of the different A cation (A= $CH_3NH_3^+$, $HC(NH_2)_2^+$, Cs^+). On the other hand, a series of computational simulation carried out using Car-Parrinello molecular dynamics, as implemented in Quantum-Espresso program package, have been

performed investigating the nature of the perovskites/TiO_2 interface, the role of moisture in the perovskite degradation process and the effect of the defect on the device working mechanism. The overall picture of our theoretical investigations underlines a crucial role of computational investigation, casting the possibility of performing predictive modeling simulations, in which the properties of a given system are simulated even before the materials laboratory synthesis and characterization. At the same time, computer simulations are shown to offer the required atomistic insight into hitherto inaccessible experimental observables.

DFT simulations of interfaces in Dye-Sensitized Solar Cells

A series of computational investigations have been carried out with the aim to set up a computational approach to accurately and reliably predict the chemical properties of the components of the DSSC (dye and nanostruttured-TiO_2) and the interaction between the photosensitizer and the semiconductor evaluating the effect of the solvent at the micro-heterogeneous interface. In particular, combined experimental and computational studies have been carried out simulating the interactions between semiconductor, organic/metallorganic molecules and liquid electrolyte. A computational approach for describing the chemical properties of the TiO_2 semiconductor has been initially calibrated. Then I moved to analyze the adsorption mode of dyes (Ruthenium- and organic dyes) on to the nanostructured TiO_2 anatase surface and the effect of the co-absorbed solvent on the geometrical and electronic properties. Moreover, the interaction between the dye-sensitized TiO_2 surface and cobalt-based electrolyte have been investigated.

Modeling ZnS and ZnO Nanostructures: Structural, Electronic, and Optical Properties

Modeling of ZnO and ZnS nanostructures material and investigating their structural, electronic and optical properties have been carried out by means of DFT/TDDFT calculations. To set up a proper comparison of the optical properties of small ZnO and ZnS clusters with the experimental results the choice of an appropriate model is mandatory since the absorption and luminescence onsets shift with the particle size due to the quantum size effect. Moreover, the nature the interaction between ZnS nanoparticles and liquid water has been studied evaluating the effect of solvation on the optical properties of these materials.

DFT and TDDFT calculation for simulating optical and electrochemical properties of Donor-Acceptor Polymers employed in Organic Photovoltaics (OPV)

A computational approach has been calibrated for describing and predicting the optical and electrochemical properties of donor-acceptor polymers employed in organic photovoltaics. Our

computational study offers a methodology for predicting the chemical properties of new polymeric material for optimizing their efficiency in the field of OPV devices.

Henry Snaith, University of Oxford, UK
Annamaria Petrozza and **Guglielmo Lanzani**, IIT POLIMI, Milano, Italy
Peng Wang, Changchun Institute of Applied Chemistry, China
Juan Bisquert, Universitat Jaume I de Castelló, Spain
Arie Zaban, Bar Ilan University, Israel
Brian O'Regan, Imperial College London, UK
Michael Grätzel and **Mohammad. K. Nazeeruddin**, EPFL, Switzerland
Emilio Palomares, ICIQ, Spain
Annabella Selloni, Princeton University, USA
Paolo Umari, Università di Padova, Italy
Silvia Picozzi, CNR-SPIN L'Aquila, Italy
Alessandro Abbotto, University Milano-Bicocca, Italy
Paolo Foggi, LENS e CNR-INO Firenze, Italy
Ralph Gebauer, ICTP Trieste, Italy
Andrea Listorti, UNIBA, Italy
Giampiero Ruani CNR-ISMN Bologna, Italy
Boualem Merabet, Djillali Liabès University, Algeria
Guido Roma, Paris-Saclay University, France

"Highly Cited Researcher" from 2018 to 2023 - Clarivate Analytics
"Premio Nasini" 2021 – Società Chimica Italiana
"Premio Feltrinelli Giovani" in Chimica – 2019 – Accademia dei Lincei
"Premio YIA2018 – Young Investigator Award 2018 – Computational Modeling, 26/09/2018 Assisi, Perugia
Scientific National Qualification **MIUR/ Italy: SC 03/B1, second level.**
Software and hardware technical Manager at CNR-SCITEC in Perugia
Member of the PhD Defense Committee of Arthur Marronnier (Polytechnique College, Paris-Saclay University, France)
Member of SCI (Società Chimica Italiana)
TUMA 2014: Pesaro, Italy, September 16-18, 2014
MRS SPRING MEETING: San Francisco, (CA) USA, April 6-10, 2015
CECAM Workshop: *Perovskite solar cells: The quest for a theoretical description.* CECAM-HQ-EPFL, Lausanne, Switzerland, August 28, 2015
HOPV 2016 Conference: Swansea, United Kingdom from 29th June to 1st July, 2016
Psi-K workshop in Rome, December 18-19, 2017
Young Investigator Award, CONFERENZA DI DIPARTIMENTO, Assisi, September 24-26, 2018
nanoGe Fall Meeting, Torremolinos, Málaga, Spain, October 22-26, 2018

International Conference on Perovskite Thin Film Photovoltaics and Perovskite Photonics and Optoelectronics (NIPHO22), Online, https://www.nanoge.org/NIPHO22/home
ICEES Riad - 2022
[illegible]
Co-organizer: CERC3 Young Chemists' workshop Modeling of Complex Systems, Perugia, from 01/05/08 to 04/05/08.
Co-organizer: HOPV 2010. Assisi, from 23/05/2010 to 27/05/2010.
Organizer: Sensitizer Activated Nanostructured Solar Cells: SANS project meeting, Perugia, from 26/09/2011 to 27/09/2011.
Organizer: CECAM Workshop: *Perovskite solar cells: The quest for a theoretical description*, CECAM-HQ-EPFL, Lausanne, Switzerland, August 28, 2015
Organizer: CONFERENZA DI DIPARTIMENTO (DSCTM-CNR) 2018 Assisi, Grand Hotel Assisi, 24-25-26 settembre.
[illegible]
Tuma 2008, L'Aquila, from 23/06/08 to 25/06/08
Tecnologia Fotovoltaica Organica Ibrida: Stato dell'Arte e Prospettive, Perugia, Sala della Partecipazione, Palazzo Cesaroni, 29/06/09
ZERO EMISSION ROME 2009, Rome, 02/10/09
Meeting FIRB03, Bologna, CNR, 26/10/09
HOPV 2010. Assisi, from 23/05/2010 to 27/05/2010.
ZERO EMISSION ROME 2010, Rome, 9/09/2010.
HOPV 2011, Valcencia, Spain, from 15/05/2011 to 18/05/2011.
TUMA 2011, University of Perugia, from 30/06/2011 to 01/07/2011.
CECAM Conference: "*Energy from the Sun: Computational Chemists and Physicists Take up the Challenge*" September 10-14, 2012 Location : Chia Laguna Resort, Cagliari, Italy.
Meso Winter Workshop: Villars, Switzerland, 16 – 19 February 2015
HOPV15 Conference: Rome, Italy, from 10 to 13 May, 2015
PSCO conference 2015: EPFL, Lausanne, Switzerland, September 27-29, 2015.
PSCO 2016: Genova, Italy, 26-28 September 2016.
PSCO 2017: Oxford, UK, 18-20 September 2017.
PSCO conference 2018: EPFL, Lausanne, Switzerland, 30 September – 2 October, 2018.
[illegible]
European master in Theoretical Chemistry and Computational Modelling (TCCM), Perugia, September 2018
European master in Theoretical Chemistry and Computational Modelling (TCCM), Perugia, September 2012
School on Numerical Methods for Materials Science Related to Renewable Energy Applications – International Center of Theoretical Physics (ICTP), Trieste, November 2012,
[illegible]
MIUR-FIRB 2003
INSTM-PRISMA 2007
Istituto Italiano di Tecnologia, Platform Computation, Project SEED 2009 "HELYOS"
FP7-NMP-2009, project 246124 "SANS'
Consiglio Nazionale delle Ricerche, Project "EFOR"
FP7-ENERGY-2010 Project "ESCORT" (contract no. 261023)
FP7-2007-2013 "MESO" Project (contract no. 604032)
H2020-LCE-2017-RES-RIA- ESPResSo - Unit Responsible
H2020-LCE-2017-RES-RIA-TwoStage-PERTPV
Project PON: BEST-4U

Project @CNR: PHOTOCAT - PI		
Name	**Institution**	**Period**
Eros Radicchi	University of Perugia, Italy	January 2017 - Today
Tom Schmitt	Northwestern University, USA	November 2018 – Today
Costanza Borghesi	University of Perugia, Italy	January 2018 – Today
Luca Gregori	University of Perugia, Italy	January 2018 – Today
Diego Sorbelli	University of Perugia, Italy	January 2018 – Today
Matteo De Santis	University of Perugia, Italy	January 2018 – Today
Damiano Ricciarelli	University of Perugia, Italy	January 2018 – Today
Miriam von Holst	KU Leuven	January 2018 – Today
Arthur Marronnier	Paris-Saclay University, France	May 2018
Nadège Marchal	Université de Mons, Belgium	March 2018
Urko Petralanda	Istituto Italiano di Tecnologia, Italy	January - February 2018
Gonzalo García-Espejo	University of Cordoba, Spain	September - December 2017
Babak Pashaei	Zanjan University, Zanjan, Iran	January - June 2017
Ali Kachmar	QEER, Qatar	June - July 2016
Daniel Sapori	CNRS, INSA de Rennes, France	May -June 2016
Ali Akbari	University of Helsinki, Finland	June 2015
Rodrigo A. Urzúa Leiva	Universidad Andrés Bello, Chile	October - December 2014
Zhang Ji	Northeast Normal University, China	October 2013 - October 2014
Laurent Lasser	Université de Mons, Belgium	November – December 2012
Joaquin Calbo	University of Valencia, Spain	December 2012

Book Chapters:

1. **Unconventional Thin Film Photovoltaics - CHAPTER 8 - First Principles Modeling of Perovskite Solar Cells: Interplay of Structural, Electronic and Dynamical Effects**; Mosconi, E.; Quarti, C.; De Angelis, F.; ISSN: Print ISBN: 978-1-78262-293-2; Year: 2016; URL: http://pubs.rsc.org/en/content/ebook/978-1-78262-293-2#!divbookcontent; Editors: Enrico Da Como, Filippo De Angelis, Henry Snaith, Alison Walker
2. **Organometal Halide Perovskite Photovoltaics: Fundamentals and Device Architectures – CHAPTER: First-principles modelling of organohalide thin films and interfaces**; Mosconi, E.; Etienne, T.; De Angelis, F.; ISSN: 978-3-319-35114-8; Year: 2016; URL: https://link.springer.com/chapter/10.1007/978-3-319-35114-8_2; Editors: Nam-Gyu Park, Michael Grätzel and Tsutomu Miyasaka
3. **Theoretical Modeling of Organohalide Perovskites for Photovoltaic Applications – CHAPTER 3: Electric Properties of Organic–Inorganic Halide Perovskites and Their Role in the Working Principles of Perovskite-Based Solar Devices**; Quarti, C.; Di Sante, D.; Tan Z. L.; Mosconi, E.; Grancini, G.; Stroppa, A.; Barone, P.; De Angelis, F.; Picozzi, S.; Rappe M. A; Year: 2016; Editors: Koichi Yamashita (The University of Tokyo, Japan) and Giacomo Giorgi for CRC-Taylor&Francis.
4. **Chapter 10 - Perovskite-based solar cells in Fundamentals, Methods, Applications and Synergy with Experimental Approaches**, Kaiser W.; Mosconi E. Edited by Garcia-Iriepa C.; Marazzi M., Theoretical and Computational Photochemistry, (2023)

Publications:

1. Mahata A.; Mosconi E.; Meggiolaro D.; Fantacci S.; De Angelis F. "Rationalizing Electron–Phonon Interactions and Hot Carriers Cooling in 2D to 3D Metal Halide Perovskites" Adv. Energy Mater., 2023, DOI: 10.1002/aenm.202303405. A+ IF=27,8
2. Hoojier R.; Weis A.; Kaiser W.; Biewald A.; Dörflinger P.; Maheu C.; Arsatiants O.; Helminger D.; Dyakonov V.; Hartschuh A.; Mosconi E.; De Angelis F.; Bein T. "Cu/Ag–Sb–I Rudorffite Thin Films for Photovoltaic Applications" Chem. Mater., 2023, DOI: 10.1021/acs.chemmater.3c01837. A IF=10,51
3. Hidalgo J.; Kaiser W.; An Y.; Li R.; Oh Z.; Castro-Méndez A.F.; LaFollette D.K.; Kim S.; Lai B.; Breternitz J.; Schorr S.; Perini C.A.R.; Mosconi E.; De Angelis F.; Correa-Baena J.P. "Synergistic Role of Water and Oxygen Leads to Degradation in Formamidinium-Based Halide Perovskites" J. Am. Chem. Soc., 2023, 145, 24549–24557. A+ IF=16,38
4. Tensi L.; Rocchigiani L.; Menendez Rodriguez G.; Mosconi E.; Zuccaccia C.; De Angelis F.; Macchioni A. "Elucidating the intimate mechanism of NAD+ hydrogenation with phosphonic acid catalysed by Cp*Ir(pyridine-2-sulfonamidate) complexes" Catal. Sci. Technol., 2023, 13, 6743.
5. Morana M.; Kaiser W.; Chiara R.; Albini B.; Meggiolaro D.; Mosconi E.; Galinetto P.; De Angelis F.; Malavasi L. "Origin of Broad Emission Induced by Rigid Aromatic Ditopic Cations in Low-Dimensional Metal Halide Perovskites" J. Phys. Chem. Lett., 2023, 14, 35, 7860–7868. A OF=6,89
6. Kollmannsberger L. K.; Poonam; Cesari C.; Khare R.; Kratky T.; Boniface M.; Tomanec O.; Michalička J.; Mosconi E.; Gagliardi A.; Günther S.; Kaiser W.; Lunkenbein T.; Zacchini S.; Warnan J.; Fischer A. R. "Mechanistic Insights into ZIF-8 Encapsulation of Atom-Precise Pt (M) Carbonyl Clusters" Chem. Mater., 2023, 35, 14, 5475–5486. IF=10,51
7. Perrotta A.; Covella S.; Russo F.; Paolumbo F.; Milella A., Armenise V.; Fracassi F.; Russo A.; Colella S.; Kaiser W.; Alothman A.A.; Mosconi E.; De Angelis F. "Plasma-Driven Atomic-Scale Tuning of Metal Halide Perovskite Surfaces: Rationale and Photovoltaic Application" Sol. RRL, 2023, 7, 2300345. IF=10,51
8. Soriano-Diaz I.; Radicchi E.; Bizzarri B.; Bizzarri O.; Mosconi E.; Ashraf Waqar M.; De Angelis F.; Nunzi F. "Modeling the Interaction of Coronavirus Membrane Phospholipids with Photocatalitically Active Titanium Dioxide" J. Phys. Chem. Lett., 2023, 14, 25, 5914–5923. IF=6,89
9. Giovilli G.; Albini B.; Grisci V.; Bonomi S.; Moroni M.; Mosconi E.; Kaiser W.; De Angelis F.; Galinetto P.; Malavasi L. "Band gap tuning through cation and halide alloying in mechanochemically synthesized Cs3(Sb1−xBix)2Br9 and Cs3Sb2(I1−xBrx)9 solid solutions" J. Mater. Chem. C., 2023, 11, 10282-10291. IF=8,07
10. Romani L.; Speltini A.; Chiara R.; Morana M.; Coccia C.; Tedesco C.; Armenise V.; Colella S.; Milella A.; Listorti A.; Profumo A.; Ambrosio F.; Mosconi E.; Pau R.; Pitzalis F.; Simbula A.; Ricciarelli D.; Saba M.; Medina-Llamas M.; De Angelis F.; Malavasi L. "Air- and water-stable and photocatalytically active germanium-based 2D perovskites by organic spacer engineering" Cell Rep. Phys. Sci. , 2023, 4, 101214. IF=7,83
11. Morelli Venturi D.; Notari M. S.; Bondi R.; Mosconi E.; Kaiser W.; Mercuri G.; Giambastiani G.; Rossin A.; Taddei M.; Costantino F. "Increased CO2 Affinity and Adsorption Selectivity in MOF-801 Fluorinated Analogues" ACS Appl. Mater. Interfaces, 2022, 14, 40801–40811. IF=9,23
12. Weis A.; Ganswindt P.; Kaiser W.; Illner H.; Maheu C.; Glück N.; Dörflinger P.; Armer M.; Dyakonov V.; Hofmann J. P.; Mosconi E.; De Angelis F.; Bein T. "Heterovalent Tin Alloying in Layered MA3Sb2I9 Thin Films: Assessing the Origin of Enhanced Absorption and Self-Stabilizing Charge States" J. Phys. Chem. C, 2022, 126, 21040–21049. IF=4,13
13. Mosconi E.; Alothman A. A.; Long R.; Kaiser W.; De Angelis F. "Intermolecular Interactions of A-Site Cations Modulate Stability of 2D Metal Halide Perovskites" ACS Energy Lett., 2023, 8, 748–752. IF=23,99 (Corresponding Author)
14. Dasgupta S.; Zuraw W.; Ahmad T.; Castriotta L. A.; Radicchi E.; Mróz W.; Ścigaj M.; Pawlaczyk L.; Tamulewicz-Szwajkowska M.; Trzciński M.; Serafińczuk J.; Mosconi E.; Di Carlo A.; De Angelis F.; Dudkowiak A.; Wojciechowski K. "Modification of a Buried Interface with Bulky Organic Cations for Highly Stable Flexible Perovskite Solar Cells" ACS Appl. Energy Mater., 2022, 5, 15114–15124. IF=6,96
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