

# Winter Workshop on Materials for Energy

WWME

2024

PROGRAM

From January 28<sup>th</sup> to February 2<sup>nd</sup> 2024  
Casa della Gioventù - University of Padova  
Brixen - Italy

<https://www.wwme2024.com/>

## *Welcome!*

It is with great pleasure that we announce the first edition of the Winter Workshop on Materials for Energy – wWME 2024, to be held in Brixen (BZ), Italy from January 28th to February 2nd.

The program will be composed by a combination of invited and contributed talks, given by established and younger scientists.

The idea is to create a connection between simulations and experiments in the field of energy harvesting in a friendly atmosphere with lots of space for networking activities.

We look forward to seeing you in Brixen!

*The Organizing Committee*

## *Invited Speakers*

Albano Cossaro (University of Trieste, IT)  
Claudia Barolo (University of Torino, IT)  
Daniele Cortecchia (University of Bologna, IT)  
Daniele Meggiolaro (CNR – SCITEC, IT)  
Elena Degoli (University of Modena&Reggio-Emilia, IT)  
Enrico Ronca (University of Perugia, IT)  
Eros Radicchi (University of Verona, IT)  
Federico Brivio (University of Perugia, IT)  
Francesca Brunetti (University of Tor Vergata, IT )  
Giovanna Bruno (University of Perugia, IT)  
Isabella Poli (IIT, IT)  
Lorenzo Monacelli (University of Roma – Sapienza, IT)  
Luca Gregori (University of Perugia, IT)  
Luca Mancini (University of Perugia, IT)  
Lucia V. Mercaldo (ENEA, IT)  
Matteo Calandra (University of Trento, IT)  
Michele Saba (University of Cagliari, IT)  
Simone Piccinin (CNR - IOM, IT)  
Udo Schwingenschlogl (KAUST, SA)  
Wldemar Kaiser (Technical University of Munich, DE)

## *Organizing Committee*

University of Perugia and Padova

Filippo De Angelis (chair)  
Paolo Umari  
Simona Fantacci  
Beatrice Bizzarri (secretary)  
Olivia Bizzarri (secretary)  
Giulia Marra (secretary)

# Winter Workshop on Materials for Energy

From January 28<sup>th</sup> to February 2<sup>nd</sup> 2024

## Day 1 - Sunday, January 28<sup>th</sup>, 2024

17:00 – 19:00	Welcome and Registration (Hotel GrunerBaum)
19:30 – 21:30	Opening Ceremony - Welcome Dinner

## Day 2 - Monday, January 29<sup>th</sup>, 2024

### Invited Lectures

08:45 – 09:00	<u>Opening</u>
<b>Session 1: Metal Halide Perovskites</b>	
09:00 – 09:30	<b>Daniele Cortecchia</b>

*“2D perovskites: a versatile chemical platform for photonic applications”*

Department of Industrial Chemistry, University of Bologna  
Center for Nanoscience and Technology, Istituto Italiano di Tecnologia, Italy

09:30 – 10:00	<b>Isabella Poli</b>
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*“Photophysics of tin halide perovskites”*

Center for Nanoscience and Technology, Istituto Italiano di Tecnologia, Italy

10:00 – 10:30	<b>Michele Saba</b>
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*“From excitons to polarons: the photophysics of lead halide perovskites”*

Department of Physics, University of Cagliari, Italy

10:30 – 11:00	<b>Daniele Meggiolaro</b>
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*“Stability and efficiency of metal halide perovskites: a computational perspective”*

Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO) Istituto  
CNR – SCITEC “Giulio Natta”, Perugia, Italy

11:00 – 11:30	<b>Luca Gregori</b>
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*“Host-dopant dative bonding facilitates molecular doping in tin-lead  
perovskites”*

Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), Istituto  
CNR – SCITEC “Giulio Natta”, Perugia, Italy  
Department of Chemistry, Biology and Biotechnology, University of Perugia,  
Italy

11:30 – 12:00	<b>Coffee Break</b>
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12:00 – 17:00	Networking
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**Session 2: Perovskite Solar cells****17:00 – 17:30****Francesca Brunetti**

*“Flexible perovskite solar cells and supercapacitors: a route towards self-powered portable and wearable electronics”*

CHOSE, Department of Electronic Engineering, University of Rome Tor Vergata, Italy

**Contribute Talks****17:30 – 17:50****Francesca De Rossi**

*“Materials and processes toward sustainable flexible perovskite solar cells”*

CHOSE, Department of Electronic Engineering, University of Rome Tor Vergata, Italy

**17:50 – 18:10****Iacopo Benesperi**

*“Copper dynamic dimers for photovoltaic applications”*

*Department of Chemistry, University of Torino, Italy  
Newcastle University, School of Nat. and Environ. Sciences, Bedson Building, Newcastle upon Tyne, UK*

**18:10 – 18:30****Giulia Folpini**

*“Understanding the excitonic properties of a sn-based 2d perovskite toward the development of light emitting devices”*

Istituto CNR – IFN, Italy  
Center for Nanoscience and Technology, Istituto Italiano di Tecnologia, Italy

18:30 – 19:30	Free - Time
19:30 – 21:30	Social Dinner

**Day 3 - Tuesday, January 30<sup>th</sup>, 2024****Invited Lectures****08:45 – 09:00****Opening****Session 1: New Methods****09:00 – 09:30****Paolo Umari**

*“TBA”*

Department of Physics and Astronomy, University of Padova, Italy

**09:30 – 10:00****Matteo Calandra***"Light induced phase transitions in thermoelectrics"*

Department of Physics, University of Trento, Italy

**10:00 – 10:30****Udo Schwingenschlögl***"Exciton dissociation by topological edge states"*

King Abdullah University of Science and Technology (KAUST), Saudi Arabia

**10:30 – 11:00****Enrico Ronca***"Using photons to control properties of molecules and materials"*

Department of Chemistry, Biology and Biotechnology (DCBB), University of Perugia, Italy

**11:00 – 11:30****Lorenzo Monacelli***"Quantum and thermal nuclear fluctuations reshape the properties of materials"*

University of Roma Sapienza, Italy

<b>11:30 – 12:00</b>	<b>Coffee Break</b>
<b>12:00 – 17:00</b>	<b>Networking</b>

**Session 2: New Methods****17:00 – 17:30****Albano Cossaro***"On-surface synthesis and characterization of boroxine molecules"*Department of Chemical and Pharmaceutical Sciences, University of Trieste, Italy  
Istituto CNR-IOM, Trieste, Italy**Contribute Talks****17:30 – 17:50****Igorann Tolbatov***"Recycling energy materials uranium and lead: insights into the bioremediation by the metal-binding proteins"*

Department of Physics and Astronomy, University of Padova, Italy

**17:50 – 18:10****Riccardo Alessandro***"Linear response equations revisited: a simple and efficient iterative algorithm"*

Department of Chemistry, Biology and Biotechnology (DCBB), University of Perugia, Italy

<b>18:10 – 19:30</b>	<b>Free - Time</b>
<b>19:30 – 21:30</b>	<b>Social Dinner</b>

Day 4 - Wednesday, January 31<sup>st</sup>, 2024

## Invited Lectures

08:45 – 09:00

Opening**Session 1: Advanced Materials**

09:00 – 09:30

Elena Degoli*“Impact of lithiation on Si-anode/binders interface for next generation lithium ions batteries”*

Department of Engineering Science and Methods, University of Modena &amp; Reggio Emilia, Italy

09:30 – 10:00

Waldemar Kaiser*“Ion migration in solid-state ion conductors from first principles and machine-learned force fields”*

Department of Physics, TUM School of Natural Sciences, Technical University of Munich, Germany

10:00 – 10:30

Lucia V. Mercaldo*“Materials, approaches, and device architectures for the challenges of photovoltaics”*

ENEA, Portici Research Center, Italy

10:30 – 11:00

Claudia Barolo*“Artificial fluorescent proteins: biophosphors for sustainable light-emitting diodes”*Department of Chemistry, NIS and INSTM Reference Centre University of Torino, Italy  
Istituto ISSMC – CNR, Italy

11:00 – 11:30

Giovanna Bruno*“Viability of hydrogen isotopes separation via quantum sieving on inexpensive alkali–earth oxides”*

Department of Chemistry, Biology and Biotechnology (DCBB), University of Perugia, Italy

11:30 – 12:00

**Coffee Break**

12:00 – 17:00

**Networking****Session 2: Advanced Materials**

17:00 – 17:30

Eros Radicchi*“Lanthanide-doped fluorides as energy-converting nanomaterials: the case of BaF<sub>2</sub>:Eu”*Nanomaterials Research Group - Department of Biotechnology, University of Verona  
INSTM, Italy

## Contribute Talks

17:30 – 17:50

Amanda Covarelli*"Developing new perovskite solar cells with machine learning methods"*

Department of Chemistry, Biology and Biotechnology (DCBB), University of Perugia, Italy

17:50 – 18:10

Tommaso Moretti*"Alkaline metal intercalation in  $TiO_2$  based anodes for new chemistry batteries"*

Department of Chemistry, Biology and Biotechnology (DCBB), University of Perugia, Italy

18:10 – 19:30

Free - Time

19:30 – 21:30

Social Dinner

Day 5 - Thursday, February 1<sup>st</sup>, 2024

## Invited Lectures

08:45 – 09:00

Opening

## Session 1: Catalysis &amp; Surfaces

09:00 – 09:30

Simone Piccinin*"Surface hole accumulation drives the oxygen evolution reaction on hematite photoanodes"*

Istituto CNR - IOM, Trieste, Italy

09:30 – 10:00

Luca Mancini*"Semi-empirical formulation of long range interactions: from small molecules to nanomaterials"*

Department of Chemistry, Biology and Biotechnology (DCBB), University of Perugia, Italy

10:00 – 10:30

Federico Brivio*"Operando modelling of  $^{27}Al$  NMR in zeolites"*

Department of Chemistry, Biology and Biotechnology (DCBB), University of Perugia, Italy

## Contribute Talks

10:30 – 10:50

Lorenzo Baldinelli*"Tailoring the electronic structure of active metals to lower the oxygen evolution reaction overpotential"*

Department of Chemistry, Biology and Biotechnology (DCBB), University of Perugia, Italy

**10:50 – 11:10****Jing Huang***"The p-type doping strategy to maintain the thermal conductivity of cubic boron arsenide"*

Beijing Computational Science Research Center, 100193 Beijing, China

<b>11:10 – 11:40</b>	<b>Coffee Break</b>
<b>11:40 – 12:00</b>	<b>Conclusion</b>
<b>12:00 – 17:00</b>	<b>Free time</b>
<b>17:00 – 18:10</b>	<b>Networking</b>
<b>18:10 – 19:30</b>	<b>Free time</b>
<b>19:30 – 21:30</b>	<b>Social Dinner</b>

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**Day 6 - Friday, February 2<sup>nd</sup>, 2024**

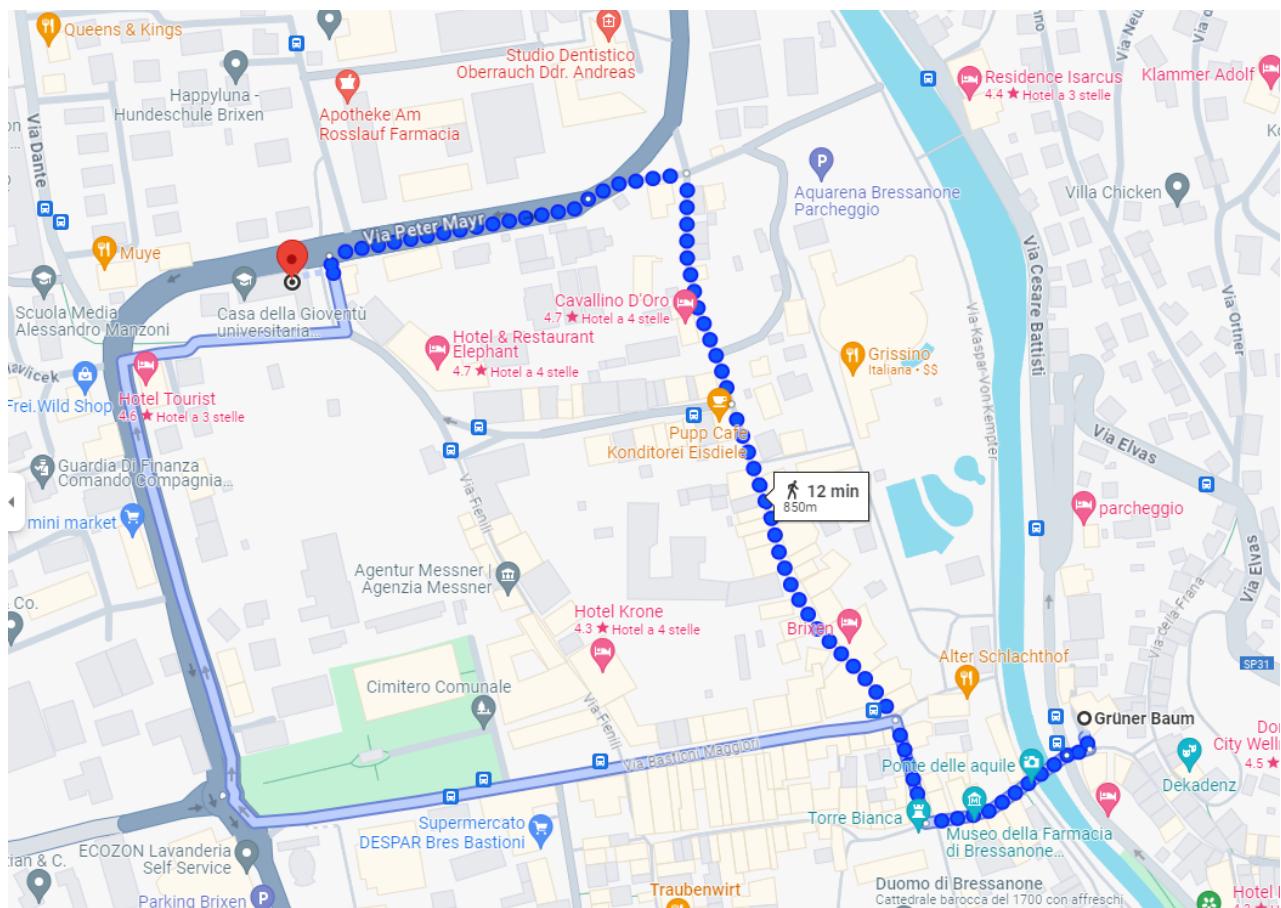
<b>09:00 – 11:35</b>	<b>SOCIAL OUTING – visit to the "Nuova Cella" Abbey (reservation required)</b>
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<b>11:35 – 12:35</b>	<b>Thanks and greetings</b>
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## Venue

The conference will be held at the Casa della Gioventù in Bressanone, a detached teaching centre of the University of Padua, which every year hosts educational and training initiatives, conferences and courses for students (including PhD students), lecturers, institutions and research facilities.

[Casa della Gioventù – via Rio Bianco, 12 – 39042 Brixen/Bressanone]



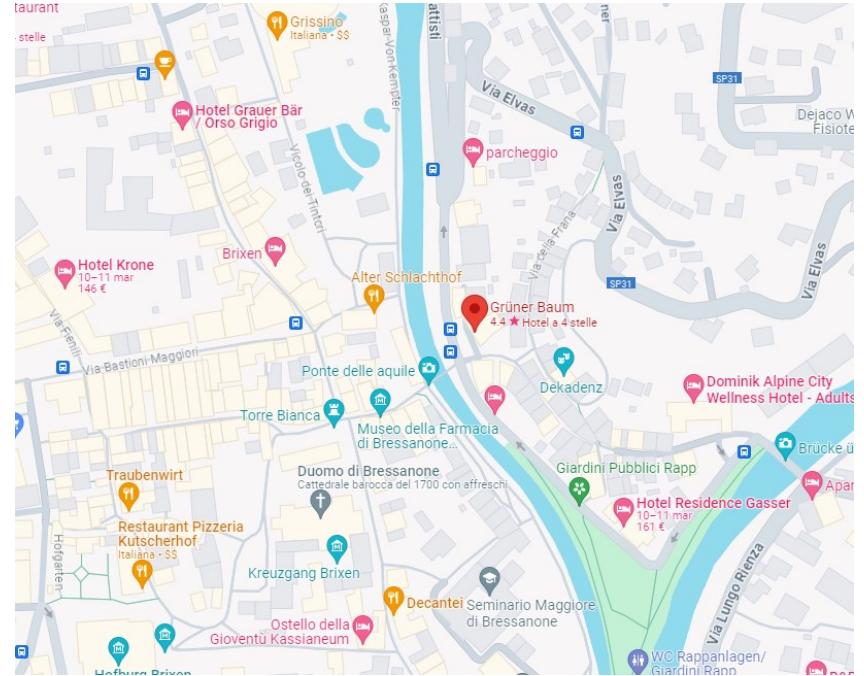
# *Social Program*

## *Welcome, and Registration*

**Sunday, Jenuary 28th, 2024**

### **Hotel GrünerBaum**

- Via Stufles, 11, 39042  
Bressanone BZ



## *Social Dinners*

**Every day**

### **Hotel GrünerBaum**

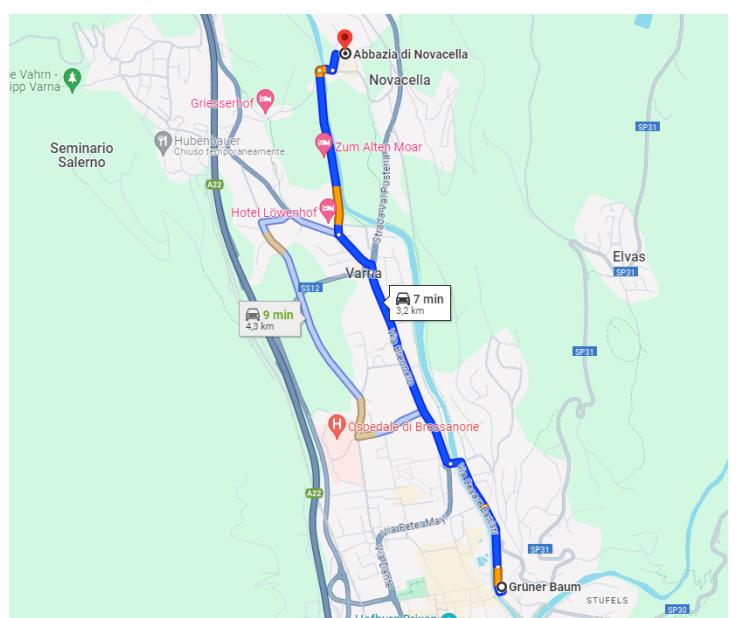
- Via Stufles, 11, 39042  
Bressanone BZ

## *Social Outing*

**Friday, February 2nd, 2024**

### **"Nuova Cella" Abbey (reservation required)**

- Via Abbazia, 1, 39040  
Novacella BZ





# Winter Workshop on Materials for Energy

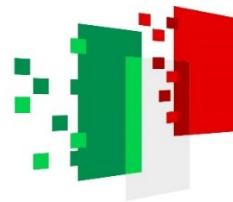
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