

Winter Workshop on Materials for Energy

WWME

**20
25**

PROGRAM

**From January 28th to February 2nd 2025
Hotel GrünerBaum
Brixen - Italy**

Welcome!

It is with great pleasure that we announce the second edition of the Winter Workshop on Materials for Energy – wWME 2025, 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 early-career 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

Giovanni Bistoni (University of Perugia, IT)
Federico Brivio (University of Padova, IT)
Francesca Brunetti (University of Rome Tor Vergata, IT)
Giovanna Bruno (University of Perugia, IT)
Matteo Calandra (University of Trento, IT)
Daniele Cortecchia (University of Bologna, IT)
Ferdinando Costantino (University of Perugia, IT)
Aldo Di Carlo (ISM-CNR, IT)
Daniele Fazzi (University of Bologna, IT)
Luca Gregori (University of Perugia, IT)
Waldemar Kaiser (Technical University of Munich, DE)
Michele Lazzeri (Sorbonne University, FR)
Isaac F. Leach (University of Perugia, IT)
Lorenzo Malavasi (University of Pavia, IT)
Massimo Mella (University of Insubria, IT)
Michele Merano (University of Padova, IT)
Lucia V. Mercaldo (ENEA, IT)
Mariachiara Pastore (CNRS, FR)
Annamaria Petrozza (IIT, IT)
Simone Piccinin (CNR-IOM, IT)
Eros Radicchi (University of Verona, IT)
Ivan Rivalta (University of Bologna, IT)
Enrico Ronca (University of Perugia, IT)
Michele Saba (Università di Cagliari, IT)
Alessandra Satta (CNR-IOM, IT)
Udo Schwingenschlögl (KAUST, SA)
Alison Walker (University of Bath, UK)

Organizing Committee

University of Perugia and Padova

Filippo De Angelis (University of Perugia, IT) (Chair)
Paolo Umari (University of Padova, IT)
Simona Fantacci (CNR-SCITEC, IT)
Federico Brivio (University of Padova, IT)
Giovanna Bruno (University of Perugia, IT)
Beatrice Bizzarri (Secretary)
Olivia Bizzarri (Secretary)
Giulia Marra (Secretary)

Winter Workshop on Materials for Energy

From January 28th to February 2nd 2025

Day 1 - Tuesday, January 28 th 2025	
18:30 – 19:00	Welcome and Registration (Hotel GrünerBaum)
20:00 – 21:30	Opening Ceremony - Welcome Dinner

Day 2 - Wednesday, January 29 th 2025	
Morning Session - Chair: Prof. Filippo De Angelis	

08:15 – 08:30 **Opening**

Invited Lectures

08:30 – 09:00 **Udo Schwingenschlögl**
"Organic Cations and Crystal Defects in Hybrid Perovskites"
 KAUST, Saudi Arabia

09:00 – 09:30 **Francesca Brunetti**
"Powering the Internet-of-Things with Perovskite Based Devices"
 University of Roma Tor Vergata, Italy

09:30 – 10:00 **Alison Walker**
"Creating a Digital Twin of a Perovskite Solar Cell"
 University of Bath, UK

10:00 – 10:30 **Michele Saba**
"Polaritons in Lead Halide Perovskites"
 University of Cagliari, Italy

Contributed Talks

10:30 – 10:50 **Tommaso Moretti**
"Perovskites: 2D or not 2D? That is the Question"
 University of Perugia, Italy

10:50 – 11:10 **Sofia Girolmoni**
"Water Repellent Low-Dimensional Perovskites for Photovoltaic Applications"
 University of Perugia, Italy

11:10 – 11:40	Coffee Break
11:40 – 17:15	Networking

Afternoon Session - Chair: Prof. Francesca Brunetti
Invited Lectures
17:15 – 17:45
Lorenzo Malavasi
"Tuning Strategies to Engineer Chiral Metal Halides"

University of Pavia, Italy

17:45 – 18:15
Luca Gregori
"Advancing Stability and Efficiency in Metal Halide Perovskites for Solar Energy Applications"

University of Perugia, Italy

18:15 – 18:45
Lucia V. Mercaldo
"Thin-Film Materials for Photovoltaics Toward High Efficiency and Integrated Solutions"

ENEA, Italy

Contributed Talks
18:45 – 19:05
Luca Angelo Betti
"High-Entropy Perovskite Oxides: Structural Stability, Solubility Limits and Catalytic Potential"

University of Pavia, Italy

19:05 – 19:25
Cesare Boriosi
"Effect of A-Site Cation on the Optoelectronic Properties of Tin Iodide Perovskites"

University of Perugia, Italy

19:25 – 19:45
Vinicius Martinelli
"C-N Cross Coupling with Nickel Bipyridine Complexes: Mechanistic Insights from Theory"

University of Perugia, Italy

19:45 – 20:00
Free Time
20:00 – 21:30
Social Dinner

Day 3 - Thursday, January 30th 2025
Morning Session - Chair: Prof. Alessandra Satta
08:25 – 08:30
Opening
Invited Lectures
08:30 – 09:00
Michele Lazzeri
"First Principles Vibrational Properties of Defected and Disordered Systems"

Sorbonne University, France

09:00 – 09:30
Simone Piccinin
"Combining Machine-Learning-Interatomic-Potentials MD and Microkinetic Modeling to Unravel the Mechanism of Photoelectrochemical Water Oxidation on Hematite"

CNR-IOM, Italy

09:30 – 10:00
Matteo Calandra
"Ultraflat Excitonic Dispersion, Half Metallicity and Band Ferromagnetism in Single Layer g-C₃N₄"

University of Trento, Italy

10:00 – 10:30
Aldo Di Carlo
"From Solution to Vacuum deposition of halide perovskite thin films for solar cell applications"

ISM-CNR, Italy

Contributed Talks
10:30 – 10:50
Giulia Fulpini
"THz Spectroscopy of Tin Perovskites: Understanding Doping and Polaronic Coupling"

IFN-CNR, Italy

10:50 – 11:10
Amanda Covarelli
"Additives in Metal-Halide Perovskite Solar Cells: a Computational Study"

University of Perugia, Italy

11:10 – 11:40
Coffee Break
11:40 – 17:15
Networking

Afternoon Session - Chair: Prof. Francesca Brunetti
Invited Lectures
17:15 – 17:45
Annamaria Petrozza
“Defects Activity in Metal Halide Perovskites”

IIT, Italy

17:45 – 18:15
Enrico Ronca
“Polaritonic Chemistry: a Field as Promising as Obscure”

University of Perugia, Italy

18:15 – 18:45
Giovanna Bruno
“Polaritonic Bloch Theorem Beyond Long-Wave Length Approximation”

University of Perugia, Italy

Contributed Talks
18:45 – 19:05
Riccardo Rossi
“Investigating the Influence of Relativistic Retardation Effects in Spin Polaritonics”

University of Perugia, Italy

19:05 – 19:25
Riccardo Alessandro
“Multireference Systems in Optical Cavities”

University of Perugia, Italy

19:25 - 19:45
Photo Group
19:45 – 20:00
Free Time
20:00 – 21:30
Social Dinner
Day 4 - Friday, January 31st 2025
Morning Session - Chair: Prof. Giovanni Bistoni
08:55 – 09:00
Opening
Invited Lectures
09:00 – 09:30
Waldemar Kaiser
“ML-Raman Calculations for Characterizing Mobile Ions in Solid-State Ion Conductors”

Technical University of Munich, Germany

09:30 – 10:00
Alessandra Satta
"Modelling the Degradation of Colors in Paintings: Exploring Potential Links to Energy Applications"

CNR-IOM, Italy

10:00 – 10:30
Massimo Mella
"Economical Processes to Separate D2 from H2: Oxides or Decorated Polycyclic Aromatic Hydrocarbons?"

University of Insubria, Italy

Contributed Talks
10:30– 10:50
Carlos Jacinto
"Novel Machine Learning Strategies for the Calculation of Relative Electronic Energies"

University of Perugia, Italy

10:50 – 11 :10
Sofia Lerda
"Shedding Light on Photocatalysis by Cobalt Complexes: a Computational Study"

University of Perugia, Italy

11:10 – 11:40
Coffee Break
11:40 – 17:15
Networking
Afternoon Session - Chair: Dr. Isaac F. Leach
Invited Lectures
17:15 – 17:45
Mariachiara Pastore
"Computational Modeling of Photoactive Materials and Interfaces for Solar Energy Conversion"

CNRS, France

17:45 – 18:15
Giovanni Bistoni
"Novel Computational Strategies for the Study of Chemical Selectivity: Combining High Accuracy and Chemical Insight"

University of Perugia, Italy

18:15 – 18:45
Isaac F. Leach
"Tools for the Rational Design of Materials: Chemical Insight from Accurate and Efficient Calculations"

University of Perugia, Italy

Contributed Talks

18:45 – 19:05
Martina Colucci

“Coupled Cluster Analysis of Intermolecular and Intramolecular Interactions in Complex Systems: from Weak Interactions to Covalent Bonds”

University of Perugia, Italy

19:05 – 19:25
Gianluca Regni

“Deciphering Resonance, Charge, and Spin Effects on London Dispersion Energy in Molecular Systems with Atomic Resolution”

University of Perugia, Italy

19:25 – 20:00	Free Time
20:00 – 21:30	Social Dinner

Day 5 - Saturday, February 1st 2025
Morning Session - Chair: Dr. Giovanna Bruno
08:25 – 08:30
Opening
Invited Lectures
08:30 – 09:00
Michele Merano

“The Out-of-Plane Optical Constant of a Two-Dimensional Crystal: Experimental Observation of an Elusive Quantity”

University of Padova, Italy

09:00 – 09:30
Federico Brivio

“Introducing ML Methods in the Dear Old DFT”

University of Perugia, Italy

09:30 – 10:00
Daniele Fazzi

“Modelling Disorder Effects in Organic Soft Materials”

University of Bologna, Italy

10:00 – 10:30
Ferdinando Costantino

“Exploiting Flexible MOFs Properties in CO₂ Adsorption and Selectivity”

University of Perugia, Italy

10:30 – 11:00
Daniele Cortecchia

“Elucidating Structure-Optical Property Relationships of Low-Dimensional Perovskites Via ssNMR Spectroscopy”

University of Bologna, Italy

11:00 – 11:30
Eros Radicchi
"An AI aided approach to materials preparation and optimization"

University of Verona, Italy

11:30 – 12:00	Coffee Break
12:00 – 17:15	Networking
17:15 – 19:00	Poster Session
19:00 – 20:00	Free time
20:00 – 21:30	Social Dinner

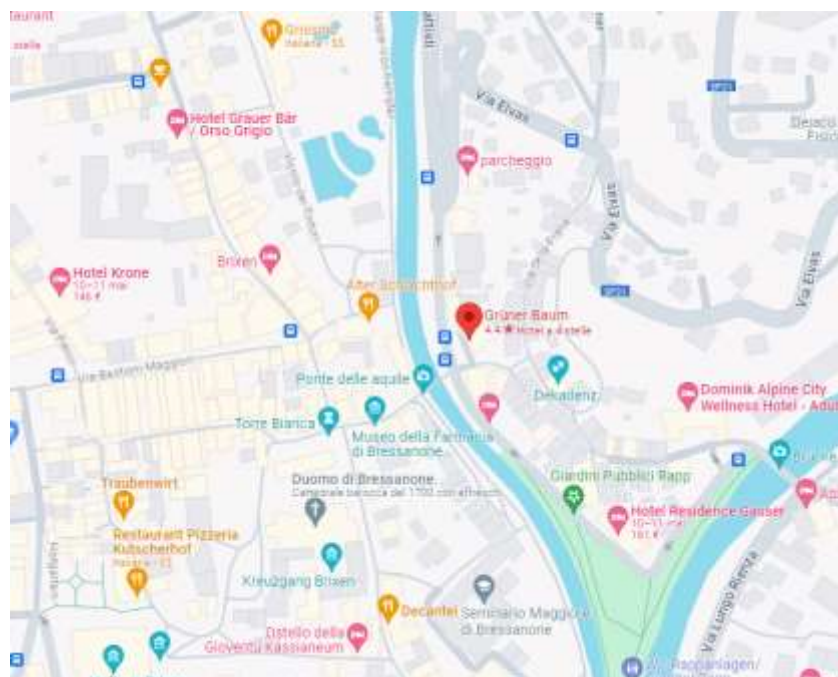
Day 6 - Sunday, February 2nd 2025

09:00 – 11:35	SOCIAL OUTING – visit to the "Novacella" Abbey (reservation required)
11:35 – 12:35	Thanks and greetings

Venue

The conference will be held at the GrünerBaum Hotel. This prestigious venue offers an ideal setting for conferences, meetings and events, combining modern facilities with the charm of the Alpine environment. The GrünerBaum Hotel regularly hosts educational and professional initiatives, making it a perfect location for this workshop.

[Hotel GrünerBaum – Via Stufles 11, 39042 Brixen/Bressanone (BZ)]



Social Program

Welcome and Registration

Sunday, January 28th, 2025

Hotel GrünerBaum

Via Stufles 11, 39042 Bressanone (BZ)

Social Dinners

Every day

Hotel GrünerBaum

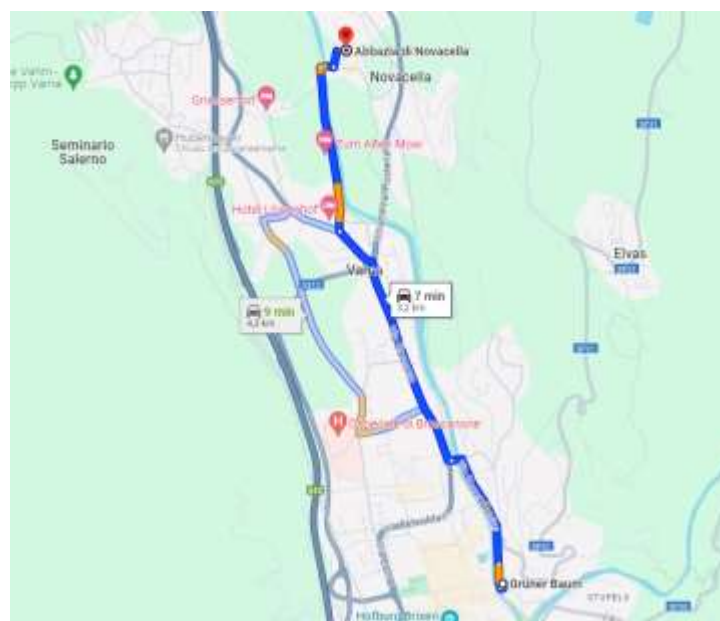
Via Stufles 11, 39042 Bressanone (BZ)

Social Outing

Sunday, February 2nd, 2025

**Novacella Abbey
(reservation required)**

Via Abbazia 1, 39040 Novacella (BZ)





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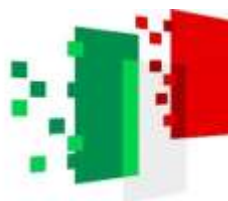
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