CALL FOR PAPERS

Abstract Deadline • October 15, 2023

CIMTEC 2024

Global Conference on

Materials in an Explosively Growing Informatics World

A cross-cutting path from materials theory, computing and data science to the hot frontiers of materials research for new informatics paradigms up to scalable quantum computing

MONTECATINI TERME, ITALY

June 20-24, 2024

CIMTEC 2024

Invitation to Attend!

The Global Conference “Materials in an Explosively Growing Informatics World” will be held on June 20-24, 2024 in Italy. The conference belongs to the highly recognized long-standing CIMTEC series of international meetings started at the end of 1960’s.

Main objectives of the Conference are:

i. to focus the latest advances and state-of-the art achievements of theoretical and computational approaches on fundamentals of materials science, processing and engineering;

ii. to evaluate and report on the state-of-the-art application of data driven accelerated discovery of new materials;

iii. to share updated theoretical studies and experimental works and to critically explore the opportunities offered by progress in materials research to further implement the overall performance of classical computers and to meet the challenges of the novel frontiers of information processing up to quantum computing.

Inorganic as well as organic materials morphologies and systems are of interest including e.g. quantum dots, nanowires, nanotubes, 2D materials, atomic clusters, extended defects, amorphous materials, crystals, polycrystalline materials, glasses, granular materials, soft condensed matter, porous media and composite, nanostructured, layered and hybrid structures.

The broad range of the subjects covered by the Conference should be very attractive for the multidisciplinary platform of mathematicians, physicists, chemists, and materials scientists and engineers working in the fields of computational materials science and computer technology.

Conference organizers are cordially inviting you to foster progress in the field by contributing to what promises to be an exciting meeting, and to enjoy the immense, unique artistic heritage and wonderful landscape of Tuscany,

Pietro Vincenzini
General Chair CIMTEC Conferences

Track A

Advances in Fundamentals of Theory, Computation and Simulation of Materials Systems: Classical to Quantum

As a tool with quantitative predictive power, cross disciplinarity and synergistic nature, computational materials science has already demonstrated its power in modelling structure and functional properties of real materials and in predicting novel materials and devices with improved performances.
However, increased ability to image and manipulate the properties of matter down to atomic scale, coupled with a deeper understanding of functions and assembly 1D, 2D and 3D nanomaterials and nano systems, is demanding further intensified efforts to develop high-fidelity theoretical and computational solutions that take into account their intrinsic behaviour.
Contributions on new achievements or refinements in theory and in computation of classical material systems and the state-of-the-art progress in theory, modelling and simulation of quantum effects in nanomaterials are encouraged. All classes of computational methods from Ab-initio and Semi empirical to Finite element methods are of interest, strong emphasis being put also on the implementation of methods bridging time and length scales across diverse orders of magnitude.

Session Topics

A-1 Ab-initio methods for bulk and reduced-dimensional materials (density functional, many-particle interacting Green's functions, quantum Monte Carlo, quantum chemistry techniques)

A-2 Quantum many-body methods for study of electron-electron and electron-phonon interactions

A-3 Molecular dynamics, Langevin dynamics, stochastic and finite element methods

A-4 Advances in multiscale computation methods, from the atomistic to the mesoscopic and continuum levels

A-5 Ultrafast excitation and decay processes in materials

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Track B

Computational Mesoscale Structure and Physico-chemical Property Evolution of Solid Materials

Focus is on the development and applications of theory and computation in combination with data science for understanding and predicting mesoscale structural and physico-chemical property evolution of materials.

Session Topics

B-1 Databases of physico-chemical properties of materials

B-2 Theory of phase transitions

B-3 Strain and size effects on phase equilibria, phase transitions, and mesoscale domain states

B-4 Structural, electric, and magnetic domain structures and their evolution under external stimuli

B-5 Thermodynamics of mesoscale states and phase transitions

B-6 Thermal, mechanical, electric, magnetic, and multifunctional properties of mesoscale structures

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Track C

Computational Tools in Materials Synthesis and Processing Science

Subject area are treatments from atomistic/mesoscopic to finite element analysis and multiscale and data-driving approaches of the wide range of physical-chemical events that are involved in the development of the structure and properties of materials during their processing, such as: self-assembly mechanisms, nanosize effects; molecular interactions, point defects and dislocations dynamics, interface and surface dynamics, phase separation and coarsening, defect/grain boundary interactions, multiple driving forces, competing kinetic mechanisms, colloidal and surface chemistry, rheology of suspensions and plastic masses, compaction, sintering, wetting and adhesion mechanisms, thermodynamics and kinetics of reaction bonding and of self-combustion and deposition processes, high pressure/shock wave/ microwave and energy beam effects…
Abstracts contributing novel design concepts, down to the atomic scale, for facilitating materials development by tackling single specific processes and mapping the relationships between structure and chemical and physical properties are welcome and will turn out especially attractive if experimentally validated.

Session Topics

Modelling and simulating phenomena and properties involved in the synthesis and fabrication of:

C-1 0D, 1D and 2D nanomaterials and nanostructures

C-2 Soft condensed matter systems

C-3 Powders, granular materials, single crystal growth

C-4 3D-bulks, composites and porous materials

C-5 Thin/thick films, layered structures and surface processing

C-6 Additive manufacturing of multiscale and multi-material structures

C-7 Data driven, machine learning to accelerate and optimize materials processing

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Special Session C-8

Exploiting Computational Tools in Materials Manufacturing and in the User Industry

Focus is on state-of-the-art computational techniques for high- throughput materials design, including computational thermodynamics and chemistry, phase field simulations, first-principle calculations, computational fluid dynamics, mechanistic modelling fusing artificial intelligence, and case studies of recent successful, practically validated use of new or commercially available software, aiding industry in improving production quality while reducing design, production time and costs and pollution. Involved are all kind of technologies for the processing and use of inorganic and organic materials from low dimensional to bulk materials and composites for the full range of functional and structural engineering applications.

Submission of abstracts is sought from academia and industry on novel single- or multiscale approach and of recently experimentally validated theoretical predictions aimed to support rationalizing or improving by computational tools, every aspect of materials manufacturing and application.

Session Topics

C-8.1 Metal and metal alloys manufacturing and user industry

C-8.2 Ceramics, glass, cement and user industry

C-8.3 Polymers and related materials and user industry

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Track D

Computer Modelling and Simulation of Materials Properties

Relevant for this Track are advances in development and application of sequential (hierarchical) or concurrent multiscale computing strategies and machine learning methods for predicting materials properties, with applications for opto-electronics, photonics, energy generation/storage and quantum information; experimental validation of computational studies. Relevant are studies that combine data- and physics-driven models for the identification of structure-property relationships and the predictive design of novel materials.

Session Topics

D-1 Materials for electronics, opto-electronics and photonics (including organic and inorganic semiconductors, halide perovskites, layered materials, soft and bio materials)

D-2 Energy generation and storage (including materials for supercapacitors, photovoltaics, thermoelectrics, ferroelectrics, piezoelectrics, batteries, osmosis, fuel cells, thermal energy)

D-3 Quantum information science (including defective solids, superconducting systems, trapped ions, magnets, molecular systems, topological defects)

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Montecatini Terme, Tettuccio

Track E

Computational Mechanics of Materials Across the Scales

A broad spectrum of theories and computational methods for the modeling and simulation of basic phenomena that control the development and behavior of the mechanical properties of materials will be covered, spanning from atomistic/mesoscopic simulations to continuum modeling, including multiscale, isogeometric, and machine-learning approaches.
Objects of analysis are advances in the theory and computation of the complex interactions and multiple phenomena occurring at the different scales contributing to mechanical properties, such as: interface properties, grain size, orientation and topology, dopants/defects accumulation at grain boundaries, crack dynamics, dislocation plasticity, glide and twinning, dislocation-precipitate interactions, phase transitions, dissipation, /quantum and transport phenomena.
Metals, metal alloys, ceramics, glasses, and polymers are of interest specifically in the form of nanowires, nanotubes, nanoshells, layered 2D nanostructures, nanocoatings, nano membranes, nanocomposites, foams, thin films and thick coatings, single crystals, crystalline and amorphous bulk materials, laminates, shells and composites under any stress/strain conditions.
This Track will cover predictions of the effects of the mechanical response of materials in engineering components subjected to a broad range of operating conditions ranging from thermomechanical equilibrium conditions, extending to cycling loading/scratching, thermal shock runs, ballistic impact, detonation loading, intense electromagnetic fields, nuclear irradiation, and reaching biochemical environments.
Abstracts of original studies contributing to advances on the above topics are welcome and will be of particular appeal if theoretical predictions are validated by tailored experiments, in view of becoming part of an integral materials-design framework.

Session Topics

E-1 Computational Mechanics of Nanoscale Materials

E-2 Computational Mechanics in Nanodevice Applications

E-3 Computational Mechanics at Mesoscopic/Macroscopic Scale

E-4 Computational Mechanics in Simulated Operating Conditions

E-5 Advances in Theory and Computational Methods

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Florence, Campanile di Giotto and Cathedral of Santa Maria del Fiore

Track F

Designing Materials for Sustainable Energy Applications

Computational materials science has already demonstrated its capability in modelling structure and functional properties for guided design of novel materials. However a more general approach to materials with predictive power of their evolution under operating conditions of realistic systems spanning diverse time and length scales is now emerging as a major challenge requiring integration of electronic, atomic, mesoscale and continuum methods, complemented by data-driving science and artificial intelligence, to establish a unified predictive framework.
This Track will highlight progress in: i-theory and multiscale modelling of the complex processes governing the behaviour of materials for energy harvesting, storage and conversion; ii-design of novel active energy materials and modelling their behaviour under simulated operating conditions.
Materials and devices for electrochemical energy conversion and storage, photovoltaics, thermoelectrics as well as solar fuels and catalysts will be covered.
Submitted abstracts on the above topics will deserve special interest if joining computation with experimental approaches.

Session Topics

F-1 Electrochemical energy systems (fuel cells, rechargeable batteries, supercapacitors; solar fuels)

F-2 Photovoltaics

F-3 Thermoelectrics

F-4 Catalysts and catalytic processes for energy applications

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Track G

Big Data, Artificial Intelligence and Machine Learning Methods for Accelerated Materials Discovery and Advancement

As we approach the new era of explosive generation of big data and creative concepts of artificial intelligence and machine learning, this Track would address virtual materials design, integration of information technology and the next generation manufacturing by identifying key challenges and opportunities for big data enhanced technologies in accelerating materials innovation to face with the needs of sustainable development and industry.
Some of key topics which will be covered are high throughput materials design and characterization, big data, materials genome and informatics, machine learning, artificial intelligence aided smart manufacturing, and other information enhanced emerging technologies.

Session Topics

G-1 Advances in machine learning principles, algorithms, descriptors and databases, machine learning approaches, their interpretability and potential pitfalls

G-2 Virtual materials design and evaluation

G-3 Integrating machine learning and simulations for materials design and manufacturing

G-4 High throughput materials characterization and testing

G-5 Big data, machine learning and artificial intelligence moving towards next generation smart manufacturing and sustainable development

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Track H

Advances in Materials and Devices Research for Digital, Neuromorphic and Unconventional Computing

Enormous progress in miniaturization and in the overall performance of classical computers has been achieved during the last several years, materials and nanotechnology being at the forefront of these exploits. However , the explosion of data that need to be processed and stored, driven by the key technologies of the fourth industrial revolution such as IOT and big data, is negatively affecting the operation speed as well as the power efficiency of the whole integrated systems in von-Neumann architecture. Research on new solutions for materials and related devices is particularly active to overcome the above limits. Merging logic and memory devices in the in-memory computing, as well as developing neuromorphic architectures and exploiting unconventional computing concepts are the new paradigms underway to assist in prospective solutions.
Progress of research in materials science, related processing technologies for advanced devices, as well as modelling and simulation of materials and device properties will be object of discussion.

Session Topics

H-1.1 Memristive materials and devices for brain inspired computing

H-1.2 Phase change materials and applications

H-2 Advances in memory and memristive devices: devices, mechanisms, and applications for computing

H-3 Neuromorphic and unconventional computing: devices, algorithms, circuits, theory

H-4 Theory, modelling and simulation of materials and devices for future computing

H-5 2D materials- and soft materials-based devices

H-6 Nanomaterials and unconventional substrates for computing

H-7 New developments in characterization methods for materials and devices

H-8 Special AFOSR Session
"From Brain-Inspired Networks for Multifunctional Systems to Neuromorphic Computing at the Edge of Biology"

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Pisa, Battistero and Torre Pendente

Track I

Towards Scalable Quantum Computing: Theory, Materials and Technology Challenges

Over the last 20 years, there has been a significant growth in the development of quantum technologies alongside advancements in classical computers. Quantum computing offers the potential to greatly surpass classical computers for certain types of problems by utilizing quantum mechanical phenomena such as superposition and entanglement. While the creation of a universal, fault-tolerant quantum computer remains a distant goal, companies and governments have recognized its potential for disruption. Many hardware platforms for quantum information processing are currently being developed and some have even been made available to the public, showing promise for a wide range of tasks including computing, simulation, networking, and sensing.

To continue advancing the performance and scalability of these devices, there is a need for a better understanding of the impact of material, interface, and surface properties, defects and imperfections on device operation and their connections to synthesis and fabrication. Additionally, new fabrication processes that are both precise and scalable are needed, as well as the exploration of new dopants such as acceptors, optically active, and high-spin nuclei dopants.

Achieving these advancements will require a tight feedback loop between characterization, imaging, theory, and simulations at the atomic scale, and synthesis and fabrication processes, as well as appropriate materials selection. It will also require the convergence of expertise from a diverse group of scientists and engineers, including those in experimental and theoretical fields.

Original papers are solicited to cover advances in physics, materials, and devices for quantum computing, including quantum state manipulation, synthesis, atomic-precision advanced manufacturing, noise control, novel characterization, and device theory and simulations, involving a wide range of qubit technologies.

Session Topics

I-1 Superconducting qubits

I-2 Defects and color centers in semiconductors

I-3 Trapped-ion, photonic and topological insulators-based qubits

I-4 Semiconductor quantum dot and dopant-based qubits

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San Gimignano

INFORMATION TO AUTHORS & PARTICIPANTS

Venue

Montecatini Terme is an internationally renown Spa and tourist resort in the environments of Florence, the historical centre of the European Renaissance. The town is placed in a strategic position to reach the most renowned historical and tourist places in Tuscany, such as Florence, Pisa, Siena, Pistoia, "Le Cinque Terre (Five Lands)", and several others.
The congress will be held at Hotel Tuscany Inn, located in the heart of Montecatini Terme, at walking distance from the hotels.

Scientific Programme

The scientific programme will consist of Plenary, Keynote, Invited Lectures and Oral and Poster contributions. English will be the official language of the conference.

Abstract Submission

Abstracts have to be submitted on-line by the *Presenting Author* and prepared according to the on-line Abstract Instructions available at the Conference web site:

www.cimtec-congress.org

Electronic submission ends on **October 15, 2023**.
Acceptance notification will be provided by December 15, 2023.
Multiple abstracts from the same *Presenting Author* are not accepted, in order to open opportunities for the broadest possible participation. Abstracts of previously unpublished matter shall only be submitted.
Abstracts of all scheduled oral and poster presentations will be made available on the conference web site to all registered participants at least 15 days in advance of the Conference.

Presentation Formats

Oral Presentations

Electronic presentation (Power Point) facilities will be available including LCD high resolution projector and PC. Cost for any special audio-visual request will be the responsibility of the individual speaker.

Poster Presentations

Authors are kindly asked to follow carefully the guidelines for Poster Preparation available at the conference web site. Attendance by at least one of the authors is requested for poster presentation.

Publication Policy

Contributions presented at CIMTEC 2024 may be submitted for publication in a special Proceedings issue of the high-quoted Elsevier-Techna Group journal CERAMICS INTERNATIONAL (Impact Factor 2022: 5.532).
All submitted papers will undergo the journal peer-review process. Proper information about submission procedures will be available in the Final Announcement.

Social Programme

The Social Programme will include various social activities. Details will be given in the Final Announcement.

Companions Programme

Guided visits to places of high historic, artistic and tourist interest will be organized. Detailed programme and registration information will be provided in the Final Announcement.

Provisional Registration

Prospective participants are kindly requested to **Pre-register** at CIMTEC 2024 website.
Presenting Authors shall not Pre-Register as they are automatically filed when submitting the Abstract.
The Final Announcement including the Provisional Programme and the information concerning registration and hotel booking will be available by February 15, 2024.

Registration Fees

Early (by April 30, 2024)

Full Member	850.00 EUR
Student	450.00 EUR

After April 30 until June 14

Full Member	920.00 EUR
Student	500.00 EUR

On site

Full Member	1000.00 EUR
Student	550.00 EUR

The Full Member and Student fees include VAT, general and secretariat costs, participation in the scientific sessions, lunches, coffees, conference bag, printed booklet of the final programme, participation in the Social Programme and Wi-Fi in the Conference venue.

Accommodation

Hotels for all pockets are available in Montecatini Terme. Half Board (HB) prices range from about 50 EUR/day for two-stars hotels to about 190.00/200.00 EUR/day for four-stars hotels. Further information and hotel booking forms will be provided with the final announcement and in the web.

Weather

The weather in Montecatini Terme in June is usually fine with temperatures ranging from 18 to 25 °C during the day and 12 to 15 °C during the night.

INFORMATION TO AUTHORS & PARTICIPANTS

Visa Application

All travel, lodging and registration expenses will be the responsibility of the individual participants. Special letters of invitation to be used for Visa application will be provided upon written request addressed well in advance to the Conference organizers, congress@technagroup.it including the following information: date of birth, place of birth, nationality, title (Ms., Mr., Dr., Prof.), affiliation, full postal address, passport number, issue and expiring dates of the passport.

How to reach Montecatini Terme

By plane:
To Florence International Airport "Amerigo Vespucci"
To Pisa International Airport "Galileo Galilei".

A complimentary bus transfer service will be arranged for CIMTEC attendees from both the Florence and Pisa Airports to Montecatini Terme on Thursday June 20 with departure from 2.00 p.m. to 12.00 p.m. CIMTEC reception hostesses will be available at the exit of arrivals terminal on June 20 (2.00 p.m to 12.00 p.m.) to assist delegates.

By train:

From Florence: train connections to Montecatini Terme are excellent and very frequent (every hour). Travel time from the Florence Central Railway Station to Montecatini Terme railway station (Montecatini Terme-Monsummano) is about 50 minutes .

From Pisa: line Pisa-Lucca, then line Lucca-Montecatini Centro. Travelling time from the Pisa Airport or downtown Pisa railway station to Montecatini Terme (via Lucca) is about 90 minutes.

By car:
Montecatini Terme can be reached easily by car from any direction via the network of Italian highways. The exit to Montecatini Terme is located midway between Florence and Pisa on the Firenze-Pisa (Florence-Pisa) express-way which is connected directly with the Central Italian expressway the "Autostrada del Sole" ("Sun Highway").

SUMMARY OF DEADLINES

October 15, 2023
Submission of Abstract

December 15, 2023
Notification of Abstract acceptance

April 30, 2024
Registration at reduced rate

INFORMATION AND CORRESPONDENCE

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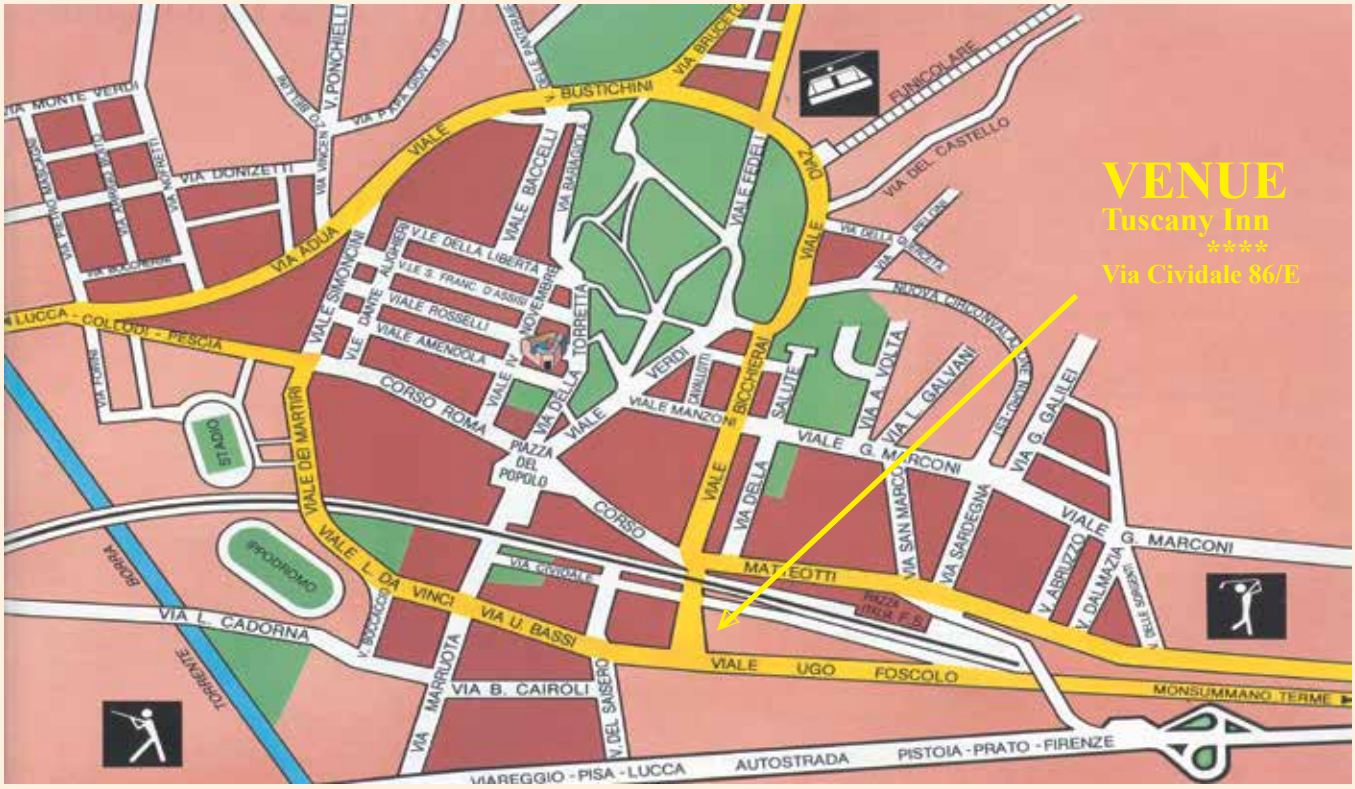


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