
# BOOK OF ABSTRACTS

The H2020 **INTERSECT** project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 814487

Organized by:

CNR NANO ISTITUTO NANOSCIENZE CONSIGLIO NAZIONALE DELLE RICERCHE

ICN2 Institut Català de Nanociència i Nanotecnologia

EXCELENCIA SEVERO OCHOA

## CONTENTS

# ORGANIZATION

## SCIENTIFIC COMMITTEE

Arrigo Calzolari – INTERSECT Project Coordinator, CNR-Nano (IT)
Nicola Marzari – INTERSECT Principal Investigator, EPFL (CH)
Andrea Padovani – INTERSECT Principal Investigator, Applied Materials Italia s.r.l. (IT)
Pablo Ordejón – INTERSECT Principal Investigator, ICN2 (ES)
Matthias Büschelberger – INTERSECT Principal Investigator, Fraunhofer IWM (DE)
Ben Kaczer – INTERSECT Principal Investigator, Imec (BE)
Johannes Ocker – INTERSECT Principal Investigator, Ferroelectric Memory Company GmbH (DE)

## ORGANIZING COMMITTEE

Arrigo Calzolari – INTERSECT Project Coordinator, CNR-Nano (IT)
Pablo Ordejón – INTERSECT Principal Investigator, ICN2 (ES)
Luisa Neri – INTERSECT Project Manager, CNR-Nano (IT)
Mara Di Berardo – INTERSECT Communication, CNR-Nano (IT)
Dámaso Torres – Graphic designer & Webmaster, ICN2 (ES)
Maria Eugenia Herrera – Competitive Funding Officer, ICN2 (ES)
Ana de la Osa Chaparro - Events and Outreach Coordinator, ICN2 (ES)

## DATE AND FORMAT

November 10-12, 2021
Hybrid live and virtual event

## VENUE

Casa Convalescència, Sant Antoni Mª Claret, 171 08041 Barcelona, Spain

# AGENDA

| CET | **Wednesday 10** |
|---|---|
| 1:30 - 2:00 pm | Welcome and opening |
| | **Session 1 - Ferroelectrics device and materials** |
| | *Session Chair: Arrigo Calzolari (CNR Nanoscience Institute)* |
| 2:00 - 2:40 pm | Sven Beyer (Global Foundries) |
| | "The FeFET – learning to handle this new powerful device available in 2x CMOS platforms" |
| 2:40 - 3:20 pm | Stefan Slesazeck (NaMLab gGmbH) |
| | "Ferroelectric tunneling junctions for beyond vonNeumann computing" |
| 3:20 - 4:00 pm | Josep Fontcuberta (Institut de Ciència de Materials de Barcelona) |
| | "Electroresistance in epitaxial HZO films" |
| 4:00 - 4:20 pm | Coffee break* |
| 4:20 - 5:00 pm | Johannes Ocker (Ferroelectric Memory GmbH) |
| | "Interplay between polarization switching and charge trapping in ferroelectric field-effect transistors" |
| 5:00 – 5:40 pm | Sergiu Clima (Imec) |
| | "Atomistic mechanisms for polarization switching and wakeup in $HFO_X$-based Ferroelectrics" |
| | "OTS material electrical parameter mapping from theoretical electronic structure" |

| CET | **Thursday 11** |
|---|---|
| | **Session 2 - Interoperability, Ontology & Workflow in Materials Modelling** |
| | *Session Chair: Pablo Ordejón (Catalan Institute of Nanoscience and Nanotechnology)* |
| 09:00 - 09:40 am | Jesper Friis (SINTEF) |
| | "Using EMMO to represent properties ontologically" |
| 09:40 - 10:20 am | Marnik Bercx and Flaviano José dos Santos (École Polytechnique Fédérale de Lausanne) |
| | "Generating a fair crystal-structure database with the AiiDA informatics platform" |
| 10:20 - 11:00 am | Matthias Büschelberger (Fraunhofer Institute for Mechanics of Materials IWM) |
| | "SimPhoNy for ontology-based material exploration" |
| 11:00 - 11:20 am | Coffee break* |
| 11:20 - 12:00 am | Emanuele Ghedini (University of Bologna) |
| | "Ontologies as a multidisciplinary approach towards data and software interoperability in applied sciences" |
| 12:00 - 12:40 pm | INTERSECT team |
| | "IM2D demonstrator" |
| 12:40 - 2:00 pm | Lunch* |

| CET | **Thursday 11** |
|---|---|
| | **Session 3 - Alternative solutions for neuromorphic computing** |
| | *Session Chair: Andrea Padovani (Applied Materials Italia)* |
| 2:00 - 2:40 pm | Daniele Ielmini (Politecnico Milano) |
| | "Recent progresses of in-memory computing: materials, devices and architectures" |
| 2:40 - 3:20 pm | Elisa Vianello (CEA-Leti) |
| | "Linking Hardware and Software for frugal AI solutions" |
| 3:20 - 4:00 pm | Mathieu Luisier (Integrated Systems Laboratory, ETH Zurich) |
| | "Ab initio Simulations of ReRAMS: from Atoms to Current vs. Voltage Characteristics" |
| 4:00 - 4:20 pm | Coffee break* |
| 4:20 - 5:00 pm | Derek Stewart (Western Digital) |
| | "Combining First Principles Simulations, Topological Constraint Theory, and Experiments to Optimize OTS Chalcogenide Alloys" |
| 5:00 - 5:40 pm | Stefano Brivio (CNR Institute for Microelectronics and Microsystems) |
| | "Memristive device optimization towards spiking neuromorphic systems" |
| 5:40 - 6:30 pm | Poster Session |
| | Social Dinner |

| CET | **Friday 12** |
|---|---|
| | **Session 4 - PCM device and materials** |
| | *Session Chair: Sergiu Clima (Imec)* |
| 09:00 - 09:40 am | Marco Bernasconi (Department of Materials Science, University of Milano-Bicocca) |
| | "Atomistic simulation of phase change materials for non-volatile memories" |
| 09:40 - 10:20 am | Andrea Padovani (Applied Materials Italia) |
| | "A Multiscale Approach to Identify Traps Responsible for Subthreshold Conduction and Threshold Switching in OTS Materials" |
| 10:20 - 11:00 am | Francesco Tavanti (CNR Nanoscience Institute) |
| | "Going deeper on the structural and electronical properties of amorphous $Ge_xSe_{1-x}$: a microscopic investigation" |
| 11:00 - 11:20 am | Coffee break* |
| 11:20 - 12:00 am | David Gao (Nanolayers Research Computing LTD) |
| | "Multiscal Materials Modelling of Nanotube-based Devices" |
| 12:00 - 12:40 pm | Nakib Protik (Catalan Institute of Nanoscience and Nanotechnology) |
| | "*ELPHBOLT* – A free Software for coupled Electron-Phonon Boltzmann Transport" |
| 12:40 - 1:30 pm | Closing |

**Room rental, coffee breaks and lunch are paid by ICN2 as co-organizer of the workshop.*

# ABSTRACTS

# SESSION 1 – FERROELECTRICS DEVICE AND MATERIALS

# THE FeFET – LEARNING TO HANDLE THIS NEW POWERFUL DEVICE AVAILABLE IN 2x CMOS PLATFORMS

Sven Beyer[1,*]

[1]Globalfoundries Inc., Dresden Module One LLC & Co. KG, Dresden, Germany
(*) sven.beyer@globalfoundries.com

With the discovery of ferroelectricity in HfO2 based thin films 2011 and the co-integration of ferroelectric field effect transistors (FeFET) into standard high-k metal gate (HKMG) CMOS platforms 2016/17 by Globalfoundries, the FeFET has emerged from a theoretical dream to an applicable reality. Maturing in the beginning as a low-cost, low power eFLASH replacement, the FeFET yet is much more than a classical stiff eNVM cell. With its great HKMG CMOS compatibility, its flexibility and its unique switching properties, it is rather to be seen as a new versatile device that promises to open up new worlds. Especially the neuromorphic design community has shifted focus towards this novel device with game-changing potential. In this talk we will discuss the actual status of GlobalFoundries FeFET technology, investigate the operation and use of this device, and discuss remaining challenges and outlook.

# FERROELECTRIC TUNNELING JUNCTIONS FOR BEYOND VONNEUMANN COMPUTING

Stefan Slesazeck[1,*], Erica Covi[1], Quang Duong[1], Suzanne Lancaster[1]

[1]NaMLab gGmbH, Noethnitzer Strasse 64 a, 01187, Dresden, Germany
(*) stefan.slesazeck@namlab.com

The discovery of ferroelectricity in doped $HfO_2$ that was firstly published in 2011 by Böschke et al. strongly increased the interest in ferroelectricity. The polarization reversal in ferroelectric $HfO_2$ films can be adopted to store information in three distinct device classes. Depending on the material stack composition different devices can be constructed from the very same ferroelectric layer - ferroelectric capacitors (FeCAP), ferroelectric field effect transistors (FeFET) and ferroelectric tunnel junctions (FTJ). The electrical characteristics of these devices are strongly influenced by the whole material stack, rather than being dictated by the properties of the ferroelectric layer itself. In this talk I will focus on the design and electrical characteristics of $HfO_2$-based FTJ bi-layer devices. Moreover, considering the application of FTJs for beyond von-Neumann architectures, I will discuss the constraints on the circuit design that arise from the specific FTJs device properties.

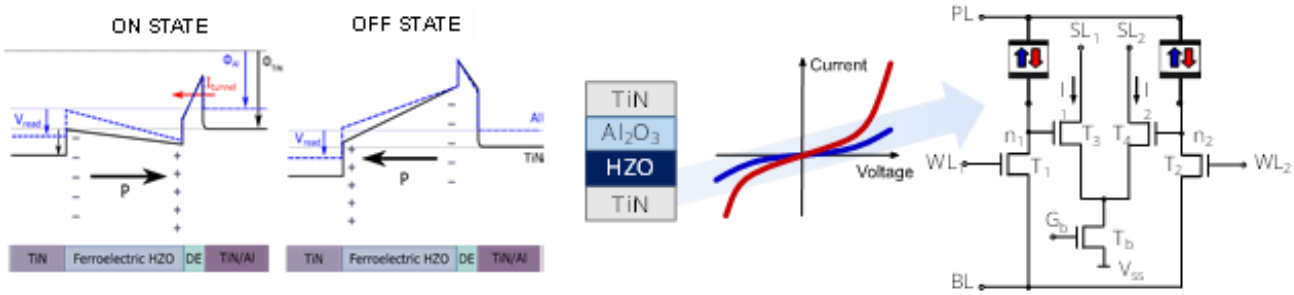



**Figure 1.** HZO/$Al_2O_3$ bi-layer Ferroelectric Tunneling Junction for adoption in differential synaptic circuit (adapted with permission from [1]. Copyright 2021 IEEE.)

**Keywords**
FTJ, ferroelectric HfO2.

**Funding**
This work was funded by the European Union's Horizon 2020 research and innovation programme under grant agreement No 871737 (www.beferrosynaptic.eu).

**Reference**
[1] E. Covi et al., "Ferroelectric Tunneling Junctions for Edge Computing", 2021 IEEE International Symposium on Circuits and Systems (ISCAS), IEEE (2021).

# ELECTRORESISTANCE IN EPITAXIAL HZO FILMS

Jacop Fontcuberta[1,*], Ignasi Fina[1]

[1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, Bellaterra, Catalonia (Spain)
(*) fontcuberta@icmab.es

Hf0.5Zr0.5O2 (HZO) ferroelectric tunnel barriers are receiving renewed attention since epitaxial thin films have become available. Indeed, epitaxial thin films have allowed reaching a deeper understanding of the role of epitaxial strain on their microstructure and its connection to the subtle balance among the different polymorphs, ferroelectric and not, of HZO. The impact of the microstructure on the electroresistance (ER) of ultrathin films is enormous. Here, I shall overview recent progress aiming to understand and tailor the phase coexistence in epitaxial films, and its relevance on measured ER, typically involving an intricate combination of genuine ferroelectric (FE) and ionic-like (IO) responses. It will be argued that suitable substrate selection allows suppressing IO-like response. Interestingly, it will also show that suitable dielectric capping allows increase the yield and endurance of tunel devices within thickness down to 1.5 nn.

**References**

[1] S. Estandía et al., ACS Appl. Electron. Mater 1, 1449−1457 (2019).
[2] M. Cervo Sulzbach et al., Adv. Electron. Mater 6, 1900852 (2020).
[3] M. Cervo Sulzbach et al., Adv. Funct. Mater 30, 2002638 (2020).
[4] Xiao Long et al., Submitted.

# INTERPLAY BETWEEN POLARISATION SWITCHING AND CHARGE TRAPPING IN FERROELECTRIC FIELD-EFFECT TRANSISTORS

Johannes Ocker[1,*], Haidi Zhou[1], Mohammad Sajedi Alvar[1], Stefan Müller[1], Andrea Padovani[2], Milan Pesic[2], Johannes Müller[3], Sven Beyer[3]

[1]Ferroelectric Memory GmbH, Dresden, Germany
[2]Applied Materials Inc., Santa Clara CA, USA
[3]Globalfoundries Dresden Module One LLC & Co. KG, Dresden, Germany
(*) Johannes.ocker@ferroelectric-memory.com

The discovery of ferroelectric hafnium oxide, which is compatible with semiconductor manufacturing, led to the re-emergence of ferroelectric field-effect transistors in modern microelectronics. Ferroelectric field effect transistors (FeFET) show unique properties for applications in the field of emerging memories, in-memory computing, and neuromorphic computing.
In order to improve FeFET device characteristics with respect to endurance, retention and variability for small device geometries, target programming algorithms can be developed. This requires a solid understanding of charge trapping and polarisation switching phenomena and their interplay in ferroelectric field-effect transistors. The switching, trapping and detrapping characteristics of the device and their influence on target programming algorithms are presented. A deep analysis on the charge trapping and polarisation switching characteristics is performed by designing comprehensive electrical tests and model the device using the GinestraTM multi-scale simulation platform.
Transfer characteristics of the FeFET devices are compared with the polarisation response of the ferroelectric capacitors (FeCAP) for better understanding of ferroelectric switching and retention mechanisms. By means of modelling the electrical characteristics it can be shown that charge trapping plays an essential part in the stabilisation of polarisation switching and can improve the retention behaviour.

**Keywords**
FeFET, Charge Trapping, Polarization Switching, Reliability.

**Funding**
Work of FMC and AMAT was funded by the EU program INTERSECT whereas the GF part was supported by the Important Project of Common European Interest (IPCEI) by the Federal Ministry of Economics and Energy and by the free state of Saxony.

**References**
[1] H. Zhou et al., “Application and Benefits of Target Programming Algorithms for Ferroelectric $HfO_2$ Transistors”, International Electron Device Conference (IEDM 2020).
[2] H. Zhou et al., “Mechanism of Retention Degradation after Endurance Cycling of $HfO_2$-based Ferroelectric Transistors”, Very Large Scale Integration Symposium (VLSI 2021).

# ATOMISTIC MECHANISMS FOR POLARIZATION SWITCHING AND WAKEUP IN $HFO_X$-BASED FERROELECTRICS

Sergiu Clima[1,*], S.R.C. McMitchell[1], B.J O'Sullivan[1], B. Kaczer,[1] G. Van den Bosch[1], G. Pourtois[1,2], J. Van Houdt[1,3]

[1]imec, Leuven, Belgium
[2]University of Antwerp, Belgium
[3]KU Leuven, Belgium
(*) sergiu.clima@imec.be

Recently, with the development of the *o*-$HfO_2$, the ferroelectrics have regained the increased interest in the device community. In an attempt to understand the atomistic mechanisms driving the polarization switching, we observe a fine balance between dipole-field energy and anion drift force that defines the switching mechanism during polarization reversal. We show that constrained relaxation can lead to 90° polarization rotation (domain deactivation). Intrinsically, the Si/$V_O$-doping can switch faster than undoped $HfO_2$ or HfZrOx.[1] By simulating the switching barrier heights in strained $HfO_2$ systems, we predict what type of crystalline structures might phase-transform during the wakeup phase of the ferroelectric operation.[2]

**Keywords**
Orthorhombic $HfO_2$, ferroelectric switching.

**References**
[1] S. Clima et al., IEDM (2020).
[2] S. Clima et al., IEDM (2018).

# OTS MATERIAL ELECTRICAL PARAMETER MAPPING FROM THEORETICAL ELECTRONIC STRUCTURE

Sergiu Clima[1,*], T. Ravsher[1,2], D.Garbin[1], A. Fantini[1], R. Degraeve[1], B. Kaczer[1], R. Delhougne[1], G. Sankar Kar[1], G. Pourtois[1,3]

[1]imec, Leuven, Belgium
[2]KU Leuven, Belgium
[3]University of Antwerp, Belgium
(*) sergiu.clima@imec.be

Large array resistive memories require a simple 2-terminal access device, so-called *selector*, in series with each memory cell in order to avoid 'sneak-path' leakage and cell misreading.[1] Ovonic Threshold Switching (OTS) materials are some of the most promising candidates for such a selector. In our endeavor to find yet undiscovered OTS materials, we investigated both theoretically (first-principles simulations)[2] and experimentally (device integration and electrical characterization)[3] a series of known OTS compositions to find theoretical-experimental parameter correlations. These correlations will help us further to screen and down select from thousands of possible elemental combinations a short-list of most promising materials to be further experimentally proven.

**Keywords**
OTS, selector.

**References**
[1] S. Clima et al., Phys. Status Solidi RRL, 1900672 (2020).
[2] F. Tavanti et al., ACS Applied Electronic Materials 2, 9, 2961 (2020).
[3] Buscemi et al., Submitted.

# SESSION 2 – INTEROPERABILITY, ONTOLOGY & WORKFLOW IN MATERIALS MODELING

# USING EMMO TO REPRESENT PROPERTIES ONTOLOGICALLY

Jesper Friis[1,*], Emanuele Ghedini[2], Gerhard Goldbeck[3], Michael Noeske[4], Thomas Hagelien[1]

[1]SINTEF, Trondheim, Norway
[2]University of Bologna, Bologna, Italy
[3]Goldbeck Consulting LTD, Cambridge, UK
[4]Fraunhofer IFAM, Bremen, Germany
(*) jesper.friis@sintef.no

When communicating measured or modelled properties within applied sciences, it is essential to also describe the conditions and boundaries under which the measurement or modelling effort was performed. The *Elemental Multiperspective Material Ontology* (EMMO), formerly known as the European Material & Modelling Ontology, starts out with exactly this in mind when formalising its description and categorisation of properties. Inspired by Pierce's semiotics, EMMO [1] describes the assignment of a property as a triadic semantic process involving the object (that possesses the property, e.g. a material sample in a measurement), a sign that stands for the property and the interpretant, which is the internal representation of the property produced by an interpreter (e.g. a measurement system).
In this presentation we will try to show how this ontological framework can be used in practice to semantically describe how physical properties are obtained and documented (e.g. whether and how they are declared, measured or modelled) and connected with a material object. We will also show how such an ontological system can be used to enable semantic interoperability in a both efficient and flexible way [2].

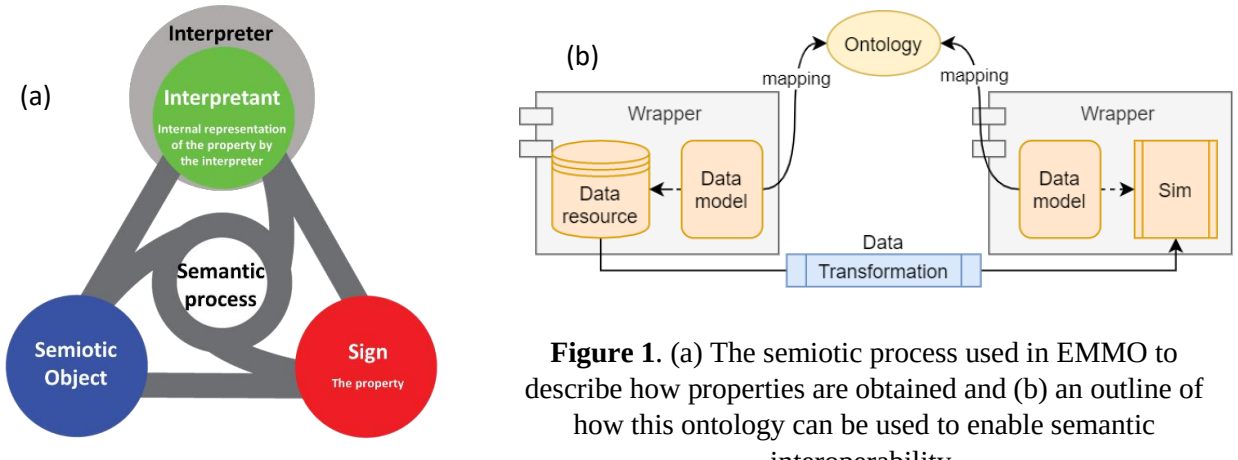



**Figure 1**. (a) The semiotic process used in EMMO to describe how properties are obtained and (b) an outline of how this ontology can be used to enable semantic interoperability.

## Keywords
Physical properties, Ontology, Interoperability.

## Funding
The authors acknowledge funding from EU's H2020 Research and Innovation Programme via the OntoTrans (862136), OpenModel (953167), and VIPCOAT (952903) projects.

## References
[1] G. Goldbeck et al., "A Reference Language and Ontology for Materials Modelling and Interoperability", NAFEMS World Congress (2019).
[2] T. Hagelien et al., "14th WCCM-ECCOMAS Congress" (2020). DOI: 10.23967/wccm-eccomas.2020.035.

# GENERATING A FAIR CRYSTAL-STRUCTURE DATABASE WITH THE AiiDA INFORMATICS PLATFORM

Marnik Bercx[1,*], Flaviano José dos Santos[1,*], Nicola Marzari[1]

[1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
(*) marnik.bercx@epfl.ch, flaviano.dossantos@epfl.ch

Computer simulations that use powerful electronic-structure techniques are widely used to characterize or predict materials' properties. Such efforts rely on databases of measured or calculated data, with structural data being especially useful. Here, we develop and validate a set of protocols to generate a comprehensive structural database of 3D materials abiding to the FAIR data principles. We start from three major experimental structure databases: the Pauling file (MPDS), the inorganic crystal structure database (ICSD), and the crystallography open database (COD). Structures are refined with density-functional theory calculations using the open-source SIRIUS accelerated library together with Quantum ESPRESSO. Since calculations are driven by the AiiDA (http://aiida.net) materials' informatics infrastructure, all curated workflows, the entire provenance of the simulations and the resulting structural data can be shared openly on the Materials Cloud (http://materialscloud.org). We present our protocols and their validation, together with the use of AiiDA's advanced automation and error handling features to create robust workflows for electronic-structure simulations. As the conductivity character of a material is unknown a-priori, we employ smearing techniques for all materials. Smearing is widely used for metallic and magnetic systems, where they improve the accuracy of Brillouin zone sampling and lessen the impact of level-crossing instabilities. Advanced smearing techniques, such as Methfessel-Paxton and Cold smearing are constructed to make the system's total free energy temperature independent at least up to the third order. In doing so, these end up with non-monotonic occupation functions (and, for Methfessel-Paxton, not positive definite), which can result in the chemical potential not being uniquely defined. Thus, we propose a protocol combining different root-finding methods to implement a data-driven solution to determine the material's correct Fermi energy. We validate the method by calculating the Fermi energy of thousands of materials and comparing them with the results of previous approaches.

**Keywords**
High-throughput, 3-D materials, Fermi energy, smearing.

**Funding**
H2020 MaX CoE Grant no. 824143.
EU H2020-NMBP-TO-IND-2018 project "INTERSECT" Grant No. 814487.

# SIMPHONY FOR ONTOLOGY-BASED MATERIAL EXPLORATION

Matthias Büschelberger[1,*], Kathrin Frei[1], Christian Eichheimer[1], Dirk Helm[1]

[1]Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstrasse 11, 79108 Freiburg, Germany
(*) matthias.bueschelberger@iwm.fraunhofer.de

At present, the increasing amount of generated data related to computational methods in material science demands for solutions that make this data findable, accessible, interoperable, and reusable (FAIR). Semantic methods, with ontologies at their core, represent a main technology to address this challenge by providing meaning to the existing data. One of their benefits is a human- and machine-readable generic material description based on natural language for the seamless exchange of knowledge between data sources.
The elementary multi-perspective material ontology (EMMO) developed by the European Material Modelling Council (EMMC) is the result of an organised multi-disciplinary effort [1] to create a base for common concepts in the field of materials modelling. In the initiative of several EU Horizon 2020 projects, the stakeholders are continuously contributing to the progress of the EMMO.
A specific EMMO-compliant solution is SimPhoNy (simulation framework for multi-scale phenomena in micro- and nanosystems), an ontology-based open-source Python framework that promotes and enables interoperability between any third-party software tools.
Such tools include the Interoperable Material-to-Device (IM2D) toolbox of the Horizon 2020-funded INTERSECT project, which furnishes semantic interoperability between simulation hub, data hub, and the graphical user interface. This is achieved through SimPhoNy by referencing the generic material science-related concepts of the ontology to the full data provenance in the data hub, while, in parallel, computations are initiated and executed in the simulation hub through AiiDA.
Besides providing semantic interpretation and cataloguing of simulation results, the ontology categorises the parametrisation into different user profiles (persona). Thereby, it gives recommendations related to the users' modelling experience without derogating the usability of the IM2D toolbox for expert users and domain specialists. Moreover, the semantic component of the IM2D toolbox enables coupling of additional workflow and backend solutions and ultimately provides the foundation for exchangeability of data between them.

**Keywords**
SimPhoNy, Ontology, Semantic Interoperability, IM2D.

**Funding**
INTERSECT (received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 814487).

**Reference**
[1] The European Materials Modelling Council on https://emmc.info/emmo-info/ (15th October 2021).

# ONTOLOGIES AS A MULTIDISCIPLINARY APPROACH TOWARDS DATA AND SOFTWARE INTEROPERABILITY IN APPLIED SCIENCES

Emanuele Ghedini[1,*]

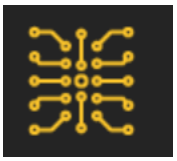
[1]Alma Mater Studiorum – Università di Bologna, Bologna, Italy
(*) emanuele.ghedini@unibo.it

In recent years there has been an increasing need for a better knowledge management in the applied sciences and industrial domains. The existence of large amount of unexploited data and the difficulties to understand, categorise and propagate such data from one domain of expertise to another is a barrier towards effective data sharing and data-driven innovation. Moreover, the lack of truly multidisciplinary platforms and methodologies that facilitates the connections between domain experts is preventing fruitful reuse of approaches and tools, acting as barrier towards cross-domain interoperability. Investigating new approaches to knowledge management to overcame such limitations requires to approach the problem through many different perspectives, questioning the traditional ways and the fundamental approaches that domain experts used up to now to deal with knowledge generation and sharing.
Ontologies (i.e. the formalization of knowledge through a logical framework) may play an important role to improve actual approaches to knowledge, being the basis for the development of interoperability framework and the gateway for human-to-machine and machine-to-human interactions, pushing towards a human centred digitalization effort. However, it is important to understand both the opportunities and the limitations of such approach and the ways in which ontologies can be used in practice to reach a factual knowledge interoperability.
After a brief introduction to ontologies, this talk will show some of the practical approaches that are actually investigated in several H2020 projects, underlining the ambitions, the current achievements and bottlenecks, following the perspectives of the European Materials Modelling Council (EMMC) and of the Elementary Multiperspective Material Ontology (EMMO), currently in development.

**Keywords**
Ontologies, Interoperability, Data, Industry 5.0.

**Funding**
The authors acknowledge funding from EU's H2020 Research and Innovation Programme via the OntoTrans (862136), OpenModel (953167), OntoCommons (958371), and SimDOME (814492) projects.

**References**
[1] G. Goldbeck et al., “A Reference Language and Ontology for Materials Modelling and Interoperability”, NAFEMS World Congress (2019).
[2] The Elementary Multiperspective Material Ontology (EMMO).



# SESSION 3 – ALTERNATIVE SOLUTIONS FOR NEUROMORPHIC COMPUTING

# RECENT PROGRESSES OF IN-MEMORY COMPUTING: MATERIALS, DEVICES AND ARCHITECTURES

D. Ielmini[1,*], F. Sancandi[1], M. Farronato[1], S. Hashemkhani[1], S. Ricci[1], M. Baldo[1], P. Mannocci[1], N. Lepri[1], L. Cattaneo[1], A. Milozzi[1], A. Glukhov[1]

[1]Dipartimento di Elettronica, Informazione e Bioingegneria, Politecnico di Milano, Italy
(*) daniele.ielmini@polimi.it

With the end of Moore's law of transistor scaling, there has been a renewed interest in unconventional concepts for computing that can overcome the memory bottleneck typical of von Neumann architectures. Among the novel computing concepts, in-memory computing (IMC) offers the opportunity of bringing computation into the memory, thus virtually suppressing data movement and the associated latency and power consumption. At the same time, IMC is also compatible with the conventional CMOS technology, is scalable and can be operated at room temperature, thus is suitable for edge computing devices and the internet of things (IoT). Figure 1 illustrates the most popular trends of IMC, including (i) accelerators of artificial neural networks, (ii) brain-inspired computing concepts and (iii) hardware accelerators for linear algebra and machine learning. While each of these topics has its own architecture and applications, they all share the fundamental requirements for high energy efficiency, high throughput and good scalability, to compete with the conventional digital CMOS technology.

This talk will review the recent progresses of IMC in terms of materials, devices and architectures. From the materials/device viewpoints, I will review novel concepts of resistive switching random access memory (RRAM) exhibiting volatile switching, thanks to the surface re-diffusion of Ag across the conductive filament. As application cases, a direction-selective IMC circuit [1] and a fully-memristive reservoir-computing circuit based on a nanowire network will be shown [2]. From the architecture viewpoint, I will present a new concept of analogue IMC with closed-loop capable of accelerating linear algebra tasks, such as matrix inverse/pseudoinverse calculation in one step [3]. The main limitations of IMC in terms of accuracy and scaling will finally be discussed.

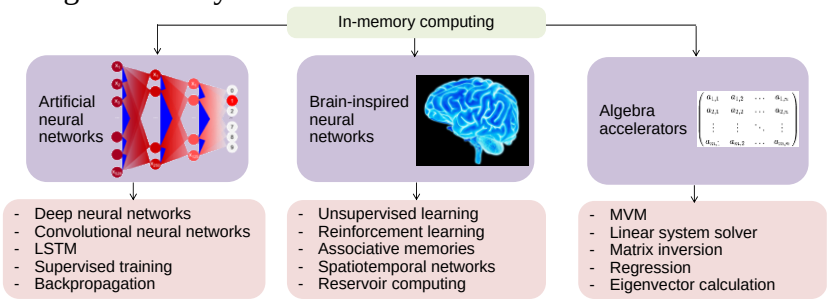



**Figure 1.** Summary of the recent trends about IMC.

**Keywords**
In-memory computing, neuromorphic computing, embedded memory, deep learning accelerators.

**References**

[1] W. Wang et al., "Neuromorphic motion detection and orientation selectivity by volatile resistive switching memories," Advanced Intelligent Systems 3, 2000224 (2020). DOI: 10.1002/aisy.202000224.

[2] G. Milano et al., "In-materia reservoir computing with a fully memristive architecture based on self-organizing nanowire networks", Nature Mater (2021). DOI: 10.1038/s41563-021-01099-9.

[3] P. Mannocci et al., "A fully-analogue, universal primitive for linear algebra operations using resistive memories", IEEE Trans. Circuits and Systems I: Regular Papers (2021).

# LINKING HARDWARE AND SOFTWARE FOR FRUGAL AI SOLUTIONS

Elisa Vianello[1,*]

[1]CEA-Leti, Grenoble, Auvergne-Rhône-Alpes, France
(*) Elisa.VIANELLO@cea.fr

Resistive random access memory (RRAM) technologies, often referred to as memristors, hold fantastic promise for implementing novel in-memory computing systems for massively parallel, low-power and low-latency computation.
This talk will first present the role of RRAM to enable the hardware implementation of Spiking Neural Networks (SNN). Second, we will present different approaches to compute in-memory with imperfect devices and without error correction codes, going from relatively conventional approaches to radical ideas exploiting device imperfections.

# AB-INITIO SIMULATIONS OF RERAMS: FROM ATOMS TO CURRENT VS. VOLTAGE CHARACTERISTICS

Mathieu Luisier[1,*], Fabian Ducry[1], Jan Aeschlimann[1], Kevin Portner[1], Christoph Weilenmann[1], Alexandros Emboras[1], Bojun Cheng[2], Juerg Leuthold[2]

[1]Integrated Systems Laboratory, ETH Zurich, Zurich, Switzerland
[2]Institute of Electromagnetic Fields, ETH Zurich, Zurich, Switzerland
(*) mluisier@iis.ee.ethz.ch

The functionality of resistive random access memories (ReRAMs) often depends on the relocation of few atoms, e.g. metallic cations in conductive bridging RAMs or oxygen vacancies in valence change memory (VCM) cells. To accurately model the behaviour of these memristive nano-devices, it is therefore important to capture the interplay between atomic positions and electrical current trajectories. An *ab-initio* quantum transport approach is ideally suited for that purpose as it can take any structure that was created, for example, through molecular dynamics (MD) or kinetic Monte Carlo (KMC) simulations as input and compute the electrical current that flows through it. Quantum mechanical tunnelling, boundary resistances, and disorder are automatically accounted for, while complex phenomena such as heat dissipation via electron relaxations and phonon emissions can also be included, but typically at high computational cost.
In this presentation I will briefly introduce the simulation framework that we developed to model ReRAM-type memristors [1] and illustrate it with two applications, namely the switching of an atomic-scale CBRAM [2] and the influence of self-heating on these devices [3]. I will also present our vision on how to integrate such computationally intensive simulations into the design flow of future ReRAMs by combining modelling tools operating at different scales.

**Keywords**
ReRAM, *ab-initio* modelling, quantum transport, multi-scale approach.

**Funding**
We acknowledge the Werner Siemens Stiftung Center for Single-Atom Electronics and Photonics and ETH Zurich under grants ETH-35 15-2 and ETH-15 19-1 for partial funding of this work as well as the Swiss National Supercomputing Centre (CSCS) under Project 971 for providing the necessary computational resources.

**References**
[1] F. Ducry, J. Aeschlimann, M. Luisier, “Electro-thermal transport in disordered nanostructures: a modeling perspective”, Nanoscale Advances 2, 2648 (2020).
[2] A. Emboras et al., “Atomic Scale Plasmonic Switch”, Nano Letters 16, 709 (2016).
[3] B. Cheng et al., “Ultra compact electrochemical metallization cells offering reproducible atomic scale memristive switching”, Communication Physics 2, Article 28 (2019).

# COMBINING FIRST PRINCIPLES SIMULATIONS, TOPOLOGICAL CONSTRAINT THEORY, AND EXPERIMENTS TO OPTIMIZE OTS CHALCOGENIDE ALLOYS

Derek A. Stewart[1,*], Kiumars Aryana[2], John Read[1], Siddarth Achar[1,3], Jim Reiner[1], Joyeeta Nag[1], Julian Schneider[4], Michael Grobis[1], Patrick Hopkins[1]

[1]Research Division, Western Digital, San Jose, USA
[2]Dept. of Mechanical and Aerospace Engineering, Univ. of Virginia, Charlottesville, USA
[3]Computational Modeling and Simulation Program, Univ. of Pittsburgh, Pittsburgh, USA
[4]Synopsys Inc., Copenhagen, Denmark
(*) derek.stewart@wdc.com

Ovonic threshold switches (OTS) based on amorphous chalcogenide alloys have emerged as leading candidates for selectors in non-volatile memory applications. The low OTS leakage current prevents sneak paths and unintentional memory cell selection. Above the threshold voltage, OTS experiences a volatile transition to a high conductivity state and provides sufficient current to switch the neighboring memory element. Given the broad interest in the switching mechanism and the nature of defects in chalcogenide glasses, there is a clear need to understand how material properties change with composition. We will highlight our work using topological constraint theory, density functional theory, and insight from experiments to identify key trends in thermal and electronic properties of chalcogenide alloys. In particular, we will show that tailoring the atomic network in $Si_xTe_{1-x}$ glasses can lead to localization of over 40% of the vibrational modes and ultralow thermal conductivity (~0.1 W/mK)[1]. Using topological constraint theory, we can link this ultralow thermal conductivity to a transition from an over-constrained (rigid) to under-constrained (floppy) atomic network for Te rich alloys. Topological constraint theory also provides a natural language to characterize the properties of multi-element chalcogenide alloys. We find that selector threshold voltage and leakage current exhibit clear trends with the mean coordination number and that this metric can be used to optimize materials[2]. Finally, given the high fields and temperatures experienced during operation, OTS/electrode interfacial interactions can significantly affect long-term device endurance. We have developed machine learning potentials[3,4] to examine interactions between GeSe alloys and Ti electrodes. Our long-term (>1 ns) molecular dynamic simulations[7] using these potentials shows significant interdiffusion at the Ti|GeSe interfaces. We will discuss the impact of interdiffusion on device performance.

**Keywords:** Chalcogenide alloys, Topological constraint theory, Phase Change, Ovonic Threshold Switch.
**Funding:** Kiumars Aryana and Siddarth Achar acknowledge funding through the Western Digital Academic Program and the WDC RAMP intern program, respectively. Work at the University of Virginia was supported in part by the NSF I/UCRC on Multi-Functional Integrated System Technology (MIST) Center IIP-1439644, IIP-1439680, and IIP1738752.

**References**

[1] K. Aryana, D. A. Stewart, J. T. Gaskin, J. Nag, J. C. Read, D. H. Olson, M. K. Grobis, P. E. Hopkins, "Tuning network topology and vibrational mode localization to achieve ultralow thermal conductivity in amorphous chalcogenides", Nature Communications 12, 2817 (2021).
[2] J. C. Read, D. A. Stewart, J. W. Reiner, B. D. Terris, "Evaluating Ovonic Threshold Switching Materials with Topological Constraint Theory", ACS Applied Materials and Interfaces 13, 37398 (2021).
[3] A. V. Shapeev, "A Class of Systematically Improvable Interatomic Potentials", Multiscale Modeling and Simulation 14, 1153 (2016).
[4] S. Smidstrup et al., "QuantumATK: an integrated platform of electronic and atomic-scale modelling tools", Journal of Physics: Condensed Matter 32, 015901 (2020).
[5] V. A. Venugopal, G. Ottaviani, C. Bersolin, D. Erbetta, A. Modelli, "Thermal stability of $Ge_2Sb_2Te_5$ in contact with Ti and TiN", Journal of Electronic Materials 38, 2063 (2009).
[6] J.-L. Battaglia, A. Kusiak, A. Saci, R. Fallica, A. Lamperti, "Effect of a thin Ti interfacial layer on the thermal resistance of $Ge_2Sb_2Te_5$-TiN stack", Applied Physics Letters 105, 121903 (2014).
[7] J. Scheider et al., "ATK-ForceField: a new generation molecular dynamics software package", Modeling Simul. Mater. Sci. Eng. 25, 085007 (2017).

# MEMRISTIVE DEVICE OPTIMIZATION TOWARDS SPIKING NEUROMORPHIC SYSTEMS

Stefano Brivio[1,*]

[1]CNR Institute for Microelectronics and Microsystems, CNR – IMM, Unit of Agrate Brianza, Agrate Brianza, Italy
(*) stefano.brivio@mdm.imm.cnr.it

Hardware spiking neural networks (SNNs) hold the great promise of a brain-inspired and efficient online processing of real-world signals impacting fields like edge-computing, robotics and prosthetics.
Resistive memory devices and memristive devices, i.e. metal/insulator/metal devices that undergo resistance change upon voltage application, have been acknowledged as key-enabling technology for hardware neural networks. In fact, they have to potential to work as synapses enabling high interconnectivity among neurons, plasticity and adaptation. However, the long-standing research on these devices have evidenced their strengths and limitations and various existing performances trade-offs. Furthermore, memristors in SNNs are used in a somewhat unconventional manner, because of system-level or algorithmic constraints.
For these reasons, it is becoming more and more evident that a co-engineering of devices and networks is needed for a breakthrough in the neuromorphic field to be fulfilled.
In this perspective, we developed non-volatile memristive devices based on $HfO_2$ layers able to show analogue plasticity evidencing strengths and limitations in their dynamics, variability and noise which are intrinsic to the physics of the operation. We further analyse these aspects in system-level by simulations of neural networks based on equation derived from CMOS circuits and real devices, thus moving some first steps towards a co-engineering of devices and systems.

**Funding**
This work is partially supported by the project Horizon 2020 EU MeM-Scales (grant No. 871371).

# SESSION 4 – PCM DEVICE AND MATERIALS

# ATOMISTIC SIMULATION OF PHASE CHANGE MATERIALS FOR NON-VOLATILE MEMORIES

O. Abou El Kheir[1], D. Dragoni[1], M. Bernasconi[1,*]

[1]Department of Materials Science, University of Milano-Bicocca, Milano, Italy
(*) marco.bernasconi@unimib.it

Phase change chalcogenide alloys are among the most promising materials for in-memory computing and for the emulation of synapses and neurons in neural network devices. These applications rest on a fast and reversible transformation between the amorphous and crystalline phases induced by Joule heating. The large difference in the electrical resistivity between the two phases enable encoding a binary, multilevel or even analogical information if partial crystallization could be controlled. The same features are exploited in phase change electronic memories (PCMs) which already entered the global market as a first example of storage class memories that combine non-volatility with access time close to that of the volatile DRAM. Materials in the same class are also investigated for embedded phase change memories operating at high temperatures for the automotive sector.
In this talk, we will discuss two recent examples on the use of electronic structure calculations to elucidate the relationship between the structure and composition of phase change alloys and their functional properties exploited in the devices. In the first example, we will discuss the results of high throughput DFT calculations aimed at tuning the composition of GeSbTe ternary alloys to raise their crystallization temperature [1]. The second example addresses the effect of confinement on the crystallization kinetics of ultrathin films of Sb which is an example of a monoatomic phase change material [2]. Large scale simulations of Sb in confined geometries have been performed by using an interatomic potential generated by fitting a large DFT database with a neural network method [3].

**Keywords**
Phase change materials; non-volatile memories; density functional theory; neural network.

**Funding**
European Union's Horizon 2020 research and innovation program under grant agreement No. 824957, project BeforeHand.

**References**
[1] O. Abou El Kheir, M. Bernasconi, "High-throughput calculations on the decomposition reactions of off-stoichiometry GeSbTe alloys for embedded memories", Nanomaterials 21, 2382 (2021).
[2] D. Dragoni, J. Behler, M. Bernasconi, "Mechanism of amorphous phase stabilization in ultrathin films of monoatomic phase change material", Nanoscale (2021). DOI: 10.1039/d1nr03432d.
[3] J. Behler, M. Parrinello, "Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces", Phys. Rev. Lett. 98, 146401 (2007).

# A MULTISCALE APPROACH TO IDENTIFY TRAPS RESPONSIBLE FOR SUBTHRESHOLD CONDUCTION AND THRESHOLD SWITCHING IN OTS MATERIALS

Andrea Padovani[1,*], Fabrizio Buscemi[1], Enrico Piccinini[1], Federico Nardi[1], Luca Larcher[1]
[1]Applied Materials Italia, Via Meuccio Ruini 72, Reggio Emilia, Italy
(*) andrea_padovani@amat.com

We propose a multiscale approach that combines experiments and device simulations to identify the active traps in chalcogenide materials for OTS application and connects them to the observed subthreshold conduction and threshold switching. The methodology relies on the accurate analysis and simulation (performed with the Ginestra® platform [1]) of carriers trapping and transport (defect-assisted, tunnelling, drift, hydrodynamic) to reproduce voltage, frequency and temperature dependence of multiple electrical characteristics, and is schematically represented in Figure 1. Figure 2 shows the excellent agreement between experiments and simulations obtained for current (I-V) and conductance (G-V) data measured on samples with 20nm-thick $Ge_{60}Se_{40}$ and $Ge_{50}Se_{50}$ films. Both devices exhibit a p-type conduction through a defect band located in the lower portion of the band-gap (compatible with Selenium vacancy traps), as seen from the extracted defect maps in Figure 2(c),(f). Moreover, the bandgap is found to reduce with the Ge content (1.45eV for $Ge_{50}Se_{50}$ and 1.1eV for $Ge_{60}Se_{40}$), in agreement with DFT results [2]. A correct characterization of GeSe traps is critical to properly model not only sub-threshold conduction, but also threshold switching. Figure 3 shows an example of current- and voltage-driven OTS characteristics simulated for a 20nm-thick $Ge_{50}Se_{50}$ device. The current-driven response (red line) highlights three different conductive regions that are self-consistently simulated considering the extracted trap properties and the developed physical model for OTS conduction (coupling trap-assisted transport, TAT, and hydrodynamic theory): 1) an OFF state at low fields due to TAT with no carrier heating; 2) a switching regime characterized by electric-field induced carrier heating (carriers fail to entirely relax their excess energy to the lattice) that allows them to sustain higher currents with lower fields, thus leading to the observed voltage-snapback; 3) a high current ON state where a hot percolation path is formed that sustains the entire current. The OTS switching modelling based on traps extracted adopting the proposed methodology well reproduces both OFF and ON states and switching voltage for GeSe films with varying composition (not shown).

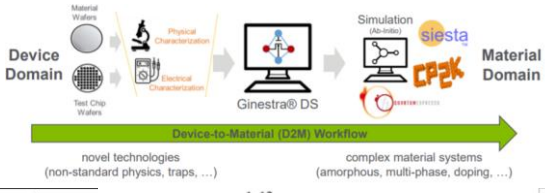



**Figure 1**. Schematic representation of the proposed methodology. (left to right) Electrical data measured on material blankets/test chips are given as input to the Ginestra® simulation platform. Experimental data are reproduced to extract relevant material parameters and trap energy/space distribution. DFT tools and material properties databases can then be used to identify the atomic structure and nature of the extracted traps.

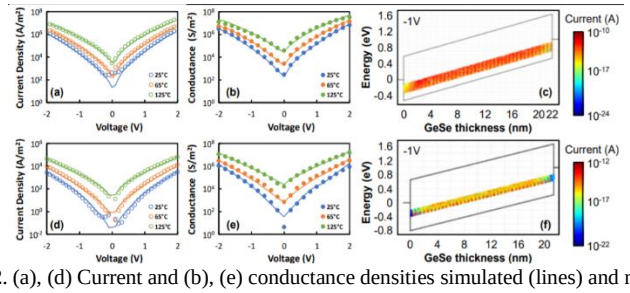



**Figure 2**. (a), (d) Current and (b), (e) conductance densities simulated (lines) and measured (symbols) at different temperatures on 20nm-thick (top row) TiN/Ge60Se40/TiN and (bottom row) TiN/Ge50Se50/TiN capacitors. (c), (f) Corresponding trap distributions as extracted by applying the proposed methodology.

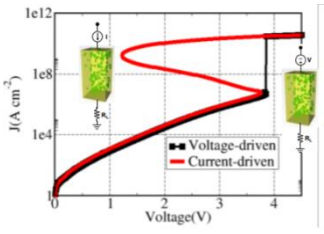



**Figure 3.** Example of J-V curves simulated for a 20nm-thick GeSe OTS under (black line) voltage-driven and (red line) current-driven modes.

**Keywords** Ginestra®, OTS switching, GeSe, trap characterization.
**Funding and Acknowledgments** The authors acknowledge financial support from the European H2020 INTERSECT project through Grant No. 814487 and thanks Ben Kaczer from imec for the experimental data.

**References**

[1] Applied Materials Ginestra®, http://www.appliedmaterials.com/products/applied-mdlxginestrasimulation-software.
[2] S. Clima, IEEE IEDM Tech. Dig., p. 4.1.1 (2017).

# GOING DEEPER ON THE STRUCTURAL AND ELECTRONICAL PROPERTIES OF AMORPHOUS $GE_XSE_{1-X}$: A MICROSCOPIC INVESTIGATION

Francesco Tavanti[1,*], Amine Slassi[1], Arrigo Calzolari[1]

[1]CNR NANO Research Center, Via Campi 213, Modena, Italy
(*) francesco.tavanti@nano.cnr.it

Amorphous chalcogenides, such as $Ge_xSe_{1-x}$, have been proposed as good ovonic switch material candidates for nonvolatile memory and selector devices due to their fast switching, endurance and higher crystallization temperature with respect to standard GST compounds. The structural and electrical properties of $Ge_xSe_{1-x}$, as for other chalcogenides, are strongly related to the presence of short- and medium-range structures in the amorphous phase that are responsible for the internal structural orders at different length-scales.[1][2]. In order to deeply understand the local geometry-dependent properties of these chalcogenides systems, we employed a combined approach based on both classical molecular dynamics (MD) simulations and density functional theory calculations.

To obtain a deep insight into the structural features of $Ge_xSe_{1-x}$ systems at the atomistic scale, MD simulations have been employed to study $Ge_xSe_{1-x}$ systems containing thousands of atoms and simulated for hundreds of nanoseconds. The obtained structures were accurately analyzed using cutting edge techniques and theories based on the chemical/physical and topological approaches shedding light on how the different percentages of Ge and Se affect the order at different lengths.

In order to compute the electronic properties of amorphous $Ge_xSe_{1-x}$ systems, we developed a procedure to extract several configurations of few hundreds of atoms from the extended structures obtained from MD simulations. The results show that a small difference in the stoichiometry affects not only the mobility band-gap size, but also the number and the position of the trap states with respect of the mobility edges.

Using both approaches, MD and quantum simulations, we obtained different information about the nature of the order in these systems demonstrating that little changes in the stoichiometry greatly affect the $Ge_xSe_{1-x}$ structural and electrical properties.

**References**

[1] F. Tavanti, B. Dianat, A. Catellani, A. Calzolari, “Hierarchical Short- and Medium-Range Order Structures in Amorphous GexSe1–x for Selectors Applications”, ACS Appl. Electron. Mater 2, 2961–2969 (2020).

[2] Z. Chai et al., “Dependence of switching probability on operation conditions in GexSe1-x ovonic threshold switching selectors”, IEEE Electron Device Letters (2019). DOI: 10.1109/led.2019.2924270.

# MULTISCALE MATERIALS MODELLING OF NANOTUBE-BASED DEVICES

D. Z. Gao[1,2,*], A.-M. El-Sayed[1], T. Durrant[1,2], A. Shluger[2], G. Bersuker[3], J. Farmer[3], Sylvester D. Olivas[3], D. Veksler[3], T. Rueckes[4], L. Cleveland[4], H. Luan[4], R. Sen[4]

[1]Nanolayers Research Computing LTD, London, UK
[2]University College London, London, UK
[3]The Aerospace Corporation, Los Angeles, USA
[4]Nantero Inc., Woburn, USA
(*) david@nanolayers.com

Carbon nanotubes (CNT) arranged in thin films have many interesting properties that make them a focus of research in a wide range of technological applications, including resistance switching and neuromorphic devices. While a single nanotube demonstrates certain desirable properties, a CNT film exhibits complex features that do not necessarily correlate to the individual tube's properties. Nevertheless, experiments show that current through a CNT film flows primarily through percolation pathways which are dependent on the structure of the film.
To model the complex behaviour of CNT films, we have taken a multi-scale approach to describe the various elements involved. Electronic structure simulations were used to calculate the current across a wide range of representative junctions between nanotubes. This data allowed us to develop simple models capable of predicting current based on the geometric properties of a nanotube pair, e.g. the minimum distance between them. On a larger scale, the film itself is treated using a mesoscopic potential, where the nanotubes are coarse-grained into connected cylindrical segments. This allows us to make representative models of CNT films with dimensions relevant to experimental devices. The current through these mesoscopic structures can be evaluated using our previously parameterized current models and compared to electrical measurements of typical devices.
The model presented here is a proof of concept, showing that the current can be directly calculated in physics-based models of CNT films. Dynamical effects can also be also included, as the films' force field allows for time-dependent evolution of the structure. Therefore, mechanisms determining device properties such as resistance switching can be identified within this model. Finally, we demonstrate how structural information and physical parameters can be extracted to be employed in statistical device simulations.

# *ELPHBOLT* - A FREE SOFTWARE FOR COUPLED ELECTRON-PHONON BOLTZMANN TRANSPORT

Nakib H. Protik[1,*], Chunhua Li[2], Miguel Pruneda[1], David Broido[2], Pablo Ordejón[1]

[1]Catalan Institute of Nanoscience and Nanotechnology – ICN2, 08193 Bellaterra, Spain
[2]Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA
(*) nakib.haider.protik@gmail.com

Accurate, parameters-free prediction of the electronic and phononic transport properties of real materials is crucial for understanding the underlying non-equilibrium physics and for identifying candidate materials for applications. In the typical approach, when the transport of one species is calculated, the other species is assumed to remain in equilibrium; i.e. the "drag effect" is ignored. It is, however, known that in certain cases the drag effect dominates the transport phenomena. We present here the Free/Libre elphbolt code which can efficiently compute the electronic and phononic transport properties using a self-consistent, *ab initio* solution of the coupled Boltzmann transport equations of the two systems. A schematic of the elphbolt workflow is shown in Figure 1.

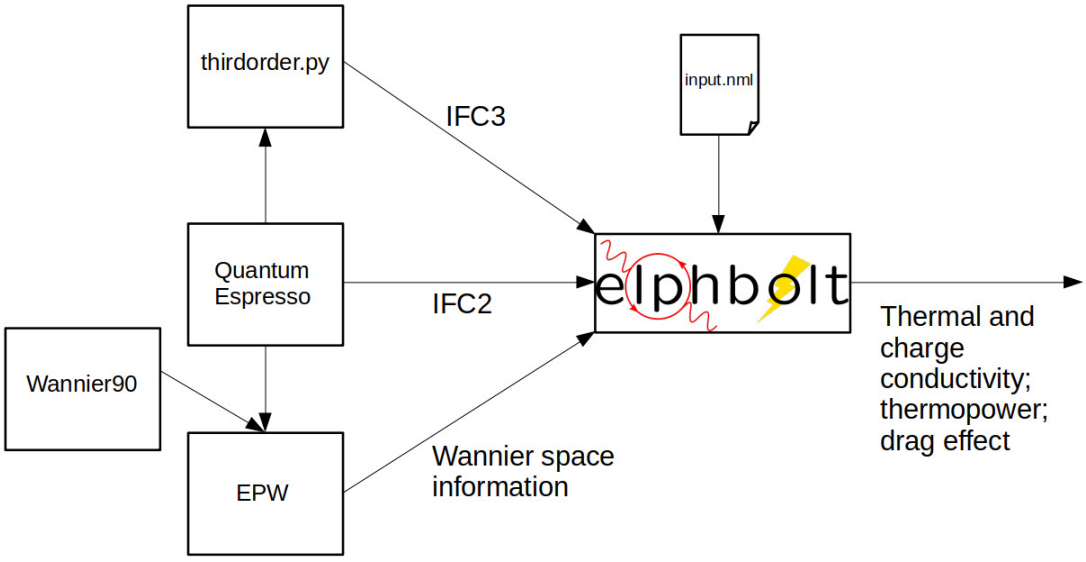
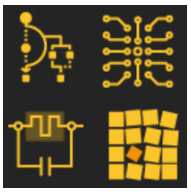



**Figure 1.** The elphbolt workflow. Real space information such as the 2nd and 3rd order force constants (IFC2 and IFC3, respectively), Wannier representations of the electronic Hamiltonian, electron-phonon interaction vertex, etc. are read from the publicly available softwares on the left. Elphbolt then computes the transport coefficients on the right following the instructions from the user.

**Keywords**
Drag effect, electron, phonon, Boltzmann transport.

**Reference(s)**

[1] N.H. Protik, Ch. Li, M. Pruneda, D. Broido, P. Ordejón. "elphbolt: An *ab initio* solver for the coupled electron-phonon Boltzmann transport equations", arXiv preprint arXiv:2109.08547 (2021).



# CONTRIBUTED ABSTRACT POSTERS

# AiiDA SIESTA BARRIER: A WORKFLOW FOR HIGH-THROUGHPUT APPROACH TO DIFFUSION IN CRYSTALS

Arsalan Akhtar[1,*], Emanuele Bosoni[2], Alberto Garcia[2], Pablo Ordejón[1], Miguel Pruneda[1]

[1]Catalan Institute of Nanoscience and Nanotechnology-ICN2, Campus UAB, 08193 Bellaterra, Spain
[2]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain
(*) arsalan.akhtar@icn2.cat

Computation of migration barriers for diffusion of small chemical species in a crystalline host is a rather complex process that requires careful consideration of a number of factors. On one side, the crystal structure of the host defines which are the possible paths that the moving species can follow.
On the other hand, the nature of the moving species (a defect in the crystal) and their interaction with its environment is also critical in determining the diffusion barriers. The development of an automatic computational framework based on the Nudged Elastic Band method (NEB) to obtain the possible diffusion energy barriers thus requires an advanced workflow scheme. Here we present a workflow implementation based on the AiiDA materials informatics platform implemented by Pizzi et al. [1] for calculating these possible diffusion paths and energy barriers with the SIESTA code [2]. The scheme identifies three main types of processes, builds the appropriate initial images for the transition path in the NEB algorithm, and calls SIESTA+NEB to extract the energetics of the corresponding migration path. The first type of process, which we label Interstitial Diffusion, is a simple jump of the moving specie from one empty interstitial site to a different interstitial position. A different scenario is possible if the moving interstitial specie takes the place of an atom in the host crystal. We label this second process as Kick Diffusion, and it leaves a substitutional defect and an intrinsic interstitial in the final lattice structure. Finally, the Exchange Diffusion takes place when two sites are swapped. A simple vacancy migration, where an atom in the host moves and fills the vacancy leaving a similar vacancy behind falls within the Exchange Diffusion process, but also an exchange of impurities, or a more complex ring exchange where three or more species are involved in the process. Our framework enables a large-scale computational high-throughput screening for studying defect mobilities and identifying new solid-state electrolytes.

**Keywords**
AiiDA, AiiDA Barriers, Diffusion, Vacancy Exchange, Exchange, Interstitial, Siesta, NEB, DFT.

**Funding**
INTERSECT (H2020-NMBP-TO-IND project GA n. 814487); Spanish MICIU, AEI and EU FEDER (Grant No. PGC2018- 096955-B-C43); Severo Ochoa program from Spanish MINECO (Grant No. SEV- 2017-0706).

**References**
[1] G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, B. Kozinsky, “AiiDA: Automated Interactive Infrastructure and Database for Computational Science”, Computational Materials Science 111, 218–230 (2016).
[2] A. Garcia et al, “Siesta: Recent developments and applications”, J. Chem. Phys. 152, 0021-9606 (2020).

# *AB INITIO* CHARACTERIZATION OF DEFECT STATES IN MATERIALS FOR NEXT-GENERATION TECHNOLOGY

Luca Bursi[1,*], Rajiv K. Chouhan[1], Alessandra Catellani[1], Arrigo Calzolari[1]

[1]CNR Nanoscience Institute, S3, Modena, Italy
(*) luca.bursi@nano.cnr.it

Information and communication technologies have been historically powered by silicon. The current major worldwide drive for big data, machine learning and quantum computing threatens to overwhelm Si-based resources and architectures. The search for alternative materials and technologies is therefore crucial and it represents a unique opportunity to explore and link materials' properties and performances in unexplored architectures.
In this upcoming process, many of the emerging candidates for next-generation technology include disrupting solutions for in-memory computing and synaptic electronics, based on chalcogenides, metal-oxides and other non-Si-based materials in their crystalline, amorphous or disordered phases [1]. Characteristic high densities of defect states play a pivotal role in transport in these systems – even more than in traditional electronics – such that defects and traps govern long-term stability and performances of devices. Therefore, describing, identifying, and controlling defect states is crucial to characterize properties of emerging materials and their interplay with non-standard device architectures, as well as to engineer already known materials through selective introduction of defects and/or dopants to improve their application range [2].
To this aim, here we focus on the study of the stability and the electronic properties of point defects in crystalline GeSe chalcogenide, which in amorphous form is proving promising for next generation electronics, and $TiO_2$, well-known material with a wide range of applications spanning form photocatalysis to electrochromic displays. The investigation has been performed by means of the Quantum ESPRESSO suite of codes [3] and of state-of-the-art high-throughput workflows for first principles condensed matter simulations, implemented mainly by Prof. Marzari's group at EPFL, in the AiiDA automated infrastructure [4], which has been actively developed, within the INTERSECT project, to handle defective systems. Our results deepen current understanding of the mechanisms underlying properties and performances of materials for next-generation technology.

**Keywords**
Defects, GeSe, $TiO_2$, ab initio-AiiDA.

**Funding**
INTERSECT Project - Interoperable Material-to-Device simulation box for disruptive electronics.

**References**
[1] M.-J. Lee et al., "A Plasma-treated chalcogenide switch device for stackable scalable 3D nanoscale memory", Nat. Commun. 4 (2013).
[2] M. Gerosa et al., "The role of defects and excess surface charges at finite temperature for optimizing oxide photoabsorbers", Nat. Mater 17, 1122 (2018).
[3] http://www.quantum-espresso.org.
[4] http://www.aiida.net.

# LATTICE THERMAL CONDUCTIVITY OF TRANSITION METAL DICHALCOGENIDES

Roberta Farris[1,*], O.Hellmann[2], K. J. Tielrooij[1], P. Ordejón[1], Z. Zanolli[3], M. J. Verstraete[4]

[1]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193, Barcelona, Spain
[2]Department of Physics, Chemistry and Biology, Linköping University, Sweden
[3]Debye Institute for Nanomaterials Science, Utrecht University, the Netherlands
[4]Université de Liège, Département de Physique, B-4000 Sart Tilman, Liège, Belgium
(*) roberta.farris@icn2.cat

Transition Metal Dichalcogenides (TMDs) are a class of materials attracting high scientific interest in recent years due to their unique properties [1]. Of particular interest is the change in electrical and optical properties with the reduction of the material thickness from bulk to monolayer [2]. Alongside electronic/optical properties, a deep understanding of the thermal properties of 2D materials and the effect of flake thickness is crucial to their implementation in devices.
In this study, we investigated the in-plane thermal conductivity (κ) and the heat capacity of TMDs,) and the heat capacity of TMDs, analyzing in detail the effect of the thickness on thermal properties and comparing with experiments. We performed first principles calculations within the density functional theory framework as implemented in the SIESTA program [3] and the Temperature Dependent Effective Potential package (TDEP) [4] for finite temperature lattice dynamics calculations. The most important novelty is the investigation of thermal properties using an ab initio approach that rigorously includes finite temperature effects, allowing to obtain room-temperature transport parameters.
By employing this method, we present a systematic study of the specific heat capacity and the thermal conductivity in TMDs at room temperature for different number of layers, from the monolayer up to the bulk structure. Our results are compared to the values measured experimentally [5].

**Keywords**
Thermal properties, phonons, DFT.

**Funding**
The author acknowledges funding from EU H2020-NMBP-TO-IND-2018 project “INTERSECT”.

**References**
[1] S.A. Han, R. Bhatia, S.W. Kim, Nano Convergence 2, 17 (2015).
[2] Y. Zhao et al., Adv. Funct. Mater. 30, 8 (2020).
[3] A. Garcia et al., J. Chem. Phys. 152, 204108 (2020).
[4] O. Hellmann, A. Abrikosov, Phys. Rev. B 88, 144301 (2013).
[5] D. Saleta et al., Submitted (2021).

# A-GeSe FOR SELECTOR MATERIALS: MODEL PREPARATION FROM FIRST-PRINCIPLES

Linda-Sheila Medondjio[1,*], He Xu[1,2], Miguel Pruneda[1], Alberto Garcia[3], Pablo Ordejon[1]

[1]Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain
[2]Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Louvain-la-Neuve, Belgium
[3]Institute of Materials Science of Barcelona (ICMAB-CSIC), Barcelona, Spain
(*) linda.medondjio@icn2.cat

The amorphous GeSe (a-GeSe) is a good candidate for the ovonic threshold switches device. Understanding of electronic property and the related structural feature is crucial for the designing and optimization of this material. The prerequisite to study the properties of amorphous materials is the identification of reliable atomic structures. To that end, we have developed realistic Density Functional Theory-based structural models of a-GeSe without resorting experimental information or adjusted interatomic potential. A series of $Ge_xSe_{1-x}$ with an extended list of stoichiometry x=0.4, 0.5, 0.6 and dopants (Si, S, As, P, Te) with various concentrations (1%, 3%, 5%,7%, 10%, 15%) has been generated with the melting-and-quenching method. The structural features, including the radial distribution function, the angle distribution function, and the coordination number distributions have been calculated. The results show that there are Ge and Se clustering in Ge and Se-rich structures, respectively; the Ge-rich structures tend to have larger coordination number, opposite to the Se-rich structures. The electronic property features, including the Crystal Orbital Hamilton Populations (COHP), inverse partition ratio (IPR), the Density of States (DOS) and the local DOS have been analyzed, and we try to identify the structural origin of these features. The mobility gap decreases with x, while in the x=0.6 samples, large numbers of in-gap localized states tend to form. The dopants behave similarly with their iso-valent hosting ions with some delicate differences, of which the structural and electronic origin has been also explored. These results will provide guide lines on the improvement of the memory switching performance of a-GeSe.

**Keywords**
Dopants, amorphous GeSe, defects, melting and quenching method.

**Funding**
BIST, Marie Curie Marie Skłodowska-Curie grant agreement No. 754558.
INTERSECT project, grant from the EU H2020-NMBP-TO-IND-2018 "Foundations for Tomorrow's Industry" call.

# THEORETICAL CHARACTERIZATION OF THE SCHOTTKY/OHMIC CONTACT BETWEEN TIN-SUBSTATE AND AMORPHOUS MATERIALS

Amine Slassi*[,1], Francesco Tavanti[1], Arrigo Calzolari[1]

[1]CNR-NANO Research Center S3, Via Campi 213/a, Modena 41125, Italy
(*) amine.slassi@nano.cnr.it

The exploitation of metallic TiN as an electrode in highly efficient electronic devices involves contact with appropriate semiconductors, where the nature of the interfacial contact plays a crucial role in controlling the device efficiency [1-2]. Here, by using first principles approaches based on the density functional theory, we systematically study the key contact properties between TiN electrode and amorphous semiconductors, including a-GeSe and a-Carbon amorphous materials that have been proposed for the realization of switching selectors in the field of synaptic electronics. Tow deposited a-GeSe amorphous thicknesses, of 1 nm and 2 nm, are considered to emulate the experimental samples. The amorphous structures are generated by using classical molecular dynamic (MD) calculations following our previous procedures [3]. Our results indicate that the interfacial contact between TiN electrode and a-GeSe is characterized by a Schottky type contact and that the Schottky barrier height (SBH) can be tuned by changing the thickness of a-GeSe slab as well as the TiN surface orientation. In contrast, the a-C almost develops an Ohmic contact in line with experimental characterizations.

**Keywords**
Ohmic contact, Schottky Contact, DFT, heterostructure, Amorphous material.

**References**

[1] A. El Haimeur, A. Slassi, A. Pershin, D. Cornil, M. Makha, E. Blanco, M. Dominguez, H. Bakkali, “Reducing p-Schottky Contact Barrier in Metal/ZnO Heterostructure Through Ni-Doping”, Applied Surface Science 545, 149023 (2021).
[2] A. Calzolari, A. Catellani, “Controlling the TiN Electrode Work Function at the Atomistic Level: A First Principles Investigation”, IEEE Access, 156308–156313 (2020).
[3] F. Tavanti, B. Dianat, A. Catellani, A. Calzolari, “Hierarchical Short- and Medium-Range Order Structures in Amorphous $Ge_xSe_{1-x}$ for Selectors Applications”, ACS Appl. Electron. Mater, 2961–2969 (2020).

# CONTACTS

**INTERSECT WORKSHOP**

E-Mail: workshop@intersect-project.eu

Website: https://intersect-workshop.icn2.cat/

**INTERSECT PROJECT**

e-mail: intersect@nano.cnr.it

website: https://intersect-project.eu/

The Book of Abstracts was edited by Mara Di Berardo, CNR-NANO.

The H2020 **INTERSECT** project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 814487