Workshop on

Digitalization and Automation Boost Energy Materials Research

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Piazzale Aldo Moro, 7 - 00185 Rome, Italy

BOOK OF ABSTRACT

Digitalization and Automation Boost Energy Materials Research

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Poster sessions

Supporting the Green Digital Transition by Digitalizing Innovative Advanced Materials: VIPCOAT, DigiPass and IAM4EU

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Abstract

The main idea of the VIPCOAT Open Innovation Platform will be presented with a focus on the co-design of innovative materials and interoperable data exchange through the digital platform. The innovation potential in developing collaboratively new active protective coatings for aeronautics along distributed production chains is considered as a demonstration example. Since VIPCOAT understands that in the end industrial players and their respective ecosystems are responsible for delivering innovations fighting todays grant challenges, the new project DigiPass built on VIPCOAT to contribute to the twin green-digital transition as a cornerstone of today's European strategy.

This transition should lead to a circular, sustainable, and net-zero-emission European economy that works for people. One basic idea of DigiPass is to pick up people working in different environments at their respective digital maturity level and to support people from day one in contributing to innovations in the area of innovative advanced materials and (intermediate) products. The DigiPass goal is to coordinate and support activities to create a sustainable digital platform that works for people and includes simultaneously assistance for Digital Materials & Product Passports and for collaborative innovation-by-design processes in a circular economy served by advanced materials.

Materials digitalization and Digital Product Passports are among the priorities included in the AMI2030 activities and considered in the IAM4EU partnership planning actions.

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Training & Knowledge Dissemination: A Case Study in Building International Networks

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Abstract

To achieve net-zero goals by 2050, Natural Resources Canada (NRCan) has supported the uptake of the accelerated materials discovery (AMD) approach for clean energy technologies in research facilities around the world. Beyond providing funding and capital and infrastructure investments, international network building for training & knowledge mobilization has been a critical component to the NRCan AMD strategy.

To that end, NRCan has led numerous initiatives such as Mission Innovation: Materials for Energy (formerly Innovation Challenge 6: Clean Energy Materials) and the German Canadian Materials Acceleration Centre (GCMAC), in part focused on educating on the AMD approach. This talk will present a case study in NRCan's approach to addressing technology specific challenges in the clean energy technology space for scale-up across the research and innovation continuum via training & knowledge mobilization, as well as connecting in with the broader ecosystem.

A Digital Framework for Adopting FAIR Principles and its Implementation in the Solar Radiation Field

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Abstract

As the field of energy research evolves, the implementation of FAIR (Findable, Accessible, Interoperable, and Reusable) principles in data management is becoming a mandatory standard. This study illustrates this implementation within the METAS dataset at the Plataforma Solar de Almería (PSA), the base of the EU-SOLARIS ERIC. Our goal is to enhance the accessibility and interoperability of solar radiation data, thereby promoting its widespread use and dissemination in the scientific community.

Since the installation of the first radiometric station at the PSA (1988), the METAS database collects all integrated solar radiation records. Recent advancements have updated its measurement capabilities to align with international quality standards. This includes the integration of advanced radiometric stations and a unique spectroradiometer system, ensuring a thorough analysis of the solar spectrum. The customised data acquisition system at METAS is crucial for high-precision data recording and management. Its integration with a FAIR-compatible management system is key to assuring data interoperability with other measurement stations around the World.

A pivotal aspect of our approach was the redesign of METAS's data and metadata structure, aligning it with global standards such as FIWARE. This reorganisation, informed by METAS's advanced measurement infrastructure, was a major step in adopting the FAIR paradigm supported by the development of a new Data Management Plan (DMP), outlining strategies for data acquisition, storage, sharing, and preservation. Moreover, the introduction of Persistent Identifiers for each data catalogue significantly enhanced data findability and traceability. Further, the ontology design was developed using a specialised vocabulary, compatible with the Data Catalog Vocabulary (DCATv2) and encoded in JSON-LD format. This ensures adherence to best data-science practices and facilitates compatibility across diverse platforms.

The implementation of this FAIR-aligned framework within the METAS system marks significant progress towards full FAIR compliance, enhancing data management in solar radiation research and establishing a new standard in energy materials research for meticulous data stewardship that can be adopted by other infrastructures. Future initiatives will focus on expanding this structured approach to additional data sources within the energy research field, further emphasising the indispensable role of FAIR principles in driving scientific innovation and collaborative research.

Demonstrating how energy data can comply with FAIR data principles avoiding large efforts and specialized skills by using csv on the web

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Abstract

While the general understanding about the need of FAIR data is increasing in academia, data governance practices largely remain unchanged. Often researchers hesitate because existing workflows for data management are routinely used and altering them would require extra efforts by individuals and collaborating teams. However, low-entry FAIR data practices exist.

This presentation shows how to easily start improving on the implementation of FAIR data principles when current workflows rely on the popular format of comma-seperated-files (csv) to organize data and feed software. We show how with the help of "csv on the web" these files can be augmented with metadata information and linked to machine-actionable standards. It is a practice for modeling tabular data recommended by the W3C internet consortium.

We show step-by-step how a csv can be transformed into a FAIR principles compliant, machine-actionable format, using an exemplary dataset to a peer-reviewed publication about Europe's Biggest Offshore Wind Farms uploaded to figshare. It is a typical data archiving upload with a number of csv files and a README to navigate potential reusers. We explain how such a file can be altered to incorporate FAIR data principles. We show how units can be made machine-factionable, how standardized vocabulary for metadata can be found and incorporated, and how the csv can take up the Dublin Core Standard to inform about authorship and licenses. The result is to complement the data containing csv files with a single text file that contains linked, additional relevant information.

Novel approaches in meta-data management and ontologies for clean energy materials

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Abstract

Clean energy transition by 2030 requires at least 10X acceleration for production-ready energy materials. The development and integration of energy materials for market-ready renewable hydrogen technology has been slow (10-15 years), resource intensive, and exhibiting an insufficient success rate. These challenges are in large part due to the poor utilization of R&D data assets. In particular, the processes of materials integration into the functional device and the testing under real conditions have been time-consuming and expensive, to a significant extent due to the lack of curated and systematic data. While there are open and extensive literature data, the stock of technical data is unstructured, un-standardized, and largely fragmented, being assembled from various experimental, synthesis, modelling and simulation sources. Reliance on unstructured and complex data (type, category, sources) compromises the effectiveness of the discovery-to-device pipeline of new materials. In this presentation, we focus on new electrochemical materials for hydrogen technologies and discuss how intelligent data management and state-of-the-art data models can empower cloud-connected labs and accelerate the device-level integration and assessment of novel materials. Innovative approaches in graph data management, AI cloud infrastructure, and deployable data models, help furnish a seamless data flow architecture to provide a unified and practically feasible modeling-characterization framework. The system can be adapted to various materials classes, characterization methods, reaction conditions and multi-step reaction procedures within the hydrogen technology field.

Fast and efficient Screening of Materials for Thermochemical Energy Storage on a novel Materials Informatics Platform

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Abstract

Finding new materials tailored for thermochemical energy storage is a crucial and challenging task, particularly in the realm of renewable energy where efficient and cost-effective materials are paramount. This is especially true for systems like batteries, fuel cells, and thermal energy storage devices, where material properties directly influence performance and cost. Traditionally, the development of new materials relies on a laborious, expensive trial-and-error approach in laboratory settings. This not only incurs high costs and slows progress, but it also carries the risk of overlooking potential material candidates or neglecting key considerations about their properties, especially in relation to their suitability for thermochemical energy storage applications and the associated business implications.

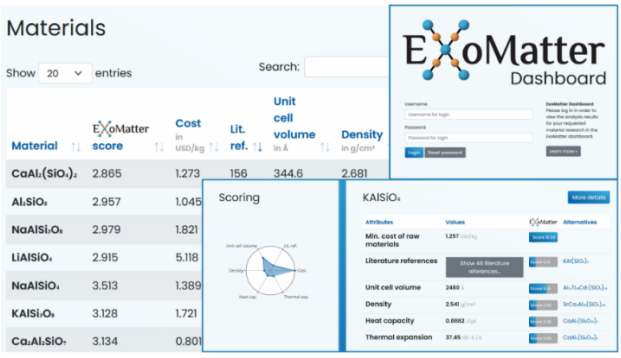

Figure 1. Screenshots of our Materials Data Platform MatterMine, featuring Scoring and Ranking functions, as well as detailed data views, literature, and patent references (https://dashboard.exomatter.ai).

Originating from research at DLR in collaboration with the Lawrence Berkeley National Laboratory ("Materials Project"), our innovative Materials Informatics solution, developed as a spin-off project from the German Aerospace Center (DLR) and subsequently commercialized as ExoMatter in 2022, addresses these challenges. [1] In our presentation, we demonstrate the integration of Density Functional Theory (DFT) calculations, Machine Learning techniques, and cost analysis to facilitate a comprehensive, multi-dimensional materials development process. Our unique scoring and ranking algorithms enable a holistic evaluation of materials, considering chemical and physical properties, sustainability, and cost factors, which are particularly critical in the context of thermochemical energy storage. We emphasize the journey from fundamental data to practical, application-specific material properties, showcasing a specific DLR case study where our methods expedited the identification of doped ceria materials for solar-thermochemical fuel production.

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IEMAP: Italian Energy Materials Acceleration Platform

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Abstract

The IEMAP project aims to create a cutting-edge digital platform designed to accelerate the discovery and selection of advanced materials for energy applications. By creating its own database and custom data management technologies, a large experimental and computational dataset can be accessed. This multidisciplinary platform leverages Big Data and artificial intelligence technologies to rapidly analyze and identify optimal materials for various energy technologies. Initial areas of focus include materials for electrochemical storage batteries, electrolyzers, and photovoltaics, key components for advancing the energy transition. The platform streamlines and simplifies the traditionally intricate and expensive processes involved in materials discovery.

At the heart of the IEMAP platform is the ENEAGRID infrastructure, powered by the CRESCO supercomputer located at ENEA's C. R. Portici. This supercomputer employs High-Performance Computing (HPC) technologies for efficient data management and the development and use of a library of numerical codes for molecular modeling. In addition, the IEMAP platform consists of several laboratories, both experimental and computational, stretching from northern to southern Italy. These laboratories, affiliated with the four main Italian research institutes - ENEA, CNR, RSE and IIT - contribute valuable data to the central hub hosted at the CRESCO supercomputer, collectively driving the progress achieved by the IEMAP platform.

Multiscale modeling of electrochemical interfaces: Challenges and chances

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Abstract

The modeling and simulation efforts on electrochemical interfaces has increased strongly in the past years related to increased focus and awareness of the energy transition, artificial intelligence and data mining, and the need for better understanding of experimental interfaces and data.

In this presentation, I want to focus on the challenges and chances of multiscale modeling of electrochemical interfaces. Firstly, I will present recent review articles discussing the challenges of modeling nanostructured materials for photocatalytic water splitting. [1,2] I will critically review where we stand at this moment. Then, I will present our multiscale, microkinetic modeling approach to investigate the limitations at electrochemical interfaces. I will manly focus on our recent example of water splitting. [3-5] Next to explaining our approach and the model, I will show recent results including sensitivity analysis. Finally, I will also touch upon earlier modeling and simulation efforts on high temperature fuel cells [6,7] and will sketch further perspectives.

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Understanding Heat Transport across Functionalized Silica-Water Interface: Insights from Molecular Dynamics Simulations

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Abstract

Thermal transport across the solid/liquid interface is crucial for numerous applications. Manipulating the heat fluxes across such interface can be essential to improve the efficiency of various heat exchange systems, insulation layer, and more generally for energy applications. In this context, the functionalization and structuration of the interface may be used to tune transfer efficiency between solid and liquid.

Silica is one of the most used materials for micro/nanofluidics. It is also present as a natural oxide layer that always exists on top of silicon, The latter being the most convenient material in optics, electronics, and micro-electro-mechanical systems. Currently, numerous studies are devoted to understanding the silica surface[1,2]. For instance, the natural passivation of the surface by different radicals, mainly by hydroxyl, was already stated[3]. At the same time, the surface functionalization by the other groups, such as methyl can be performed if a hydrophobic behavior is required. The ratio between these groups' concentrations can significantly modify the wetting characteristics of silica surfaces.

This motivates the investigation of the influence of these radicals on thermal transport perturbations across a silica/water interface with molecular dynamics simulations. To tackle this goal, firstly, we considered wetting characteristics and adhesion of a silica surface functionalized by the hydroxyl and methyl groups, varying their concentration. Further, the interfacial boundary resistance was calculated across an interface made of water and functionalized silica. In order to accurately catch the physical insights of the functionalization impact on the heat flux perturbations, we decompose the contribution of each atom group on the integral heat flux. These data were correlated with the contribution of these groups in the total work of adhesion. Our study is essential for developing a strategy for conceptualizing novel heat exchange systems based on the atomistic mechanisms of thermal transport.

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Multi-physics COMSOL Simulation of Five Heat Generation Factors in Photovoltaic Devices

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Abstract

Recently, 3D simulation platforms have been introduced, featuring sophisticated models capable of coupling optical-electrical-thermal modules to analyze the different aspect of energy devices. Even though solar cells operate as thermodynamic devices, the mechanisms of heat generation and dissipation within these devices have received limited investigation, particularly in the context of modeling and multi-physics simulation analysis. In these scenarios, the thermodynamics of the cell can exert a profound impact, potentially limiting the device's operation and stability. Factors such as selfhealing processes related to surface and bulk non-radiative recombination and heat generation due to light absorption (thermalization) play critical roles in this context. Consequently, it is imperative to conduct a thorough analysis of the heat generation factors and their influence on device characteristics. Such an analysis is essential for devising strategies to maintain a delicate balance between heat generation and dissipation within the solar cell to ensure optimal and reliable operation.

A multi-physics coupled model has been developed in COMSOL simulation package which considers five distinct heat generation factors: Thermalization, Joule heat, Peltier heat, Surface Recombination heat, and non-radiative recombination heat (comprising Shockley-Read-Hall and Auger processes).

Simulation results (Fig. 1) shows that Thermalization emerges as the dominant heat generation factor in solar cells regardless of the applied voltage. Conversely, non-radiative recombination heat and Joule heat exhibit a voltage-dependent behavior. In addition, surface recombination heat is higher at opencircuited voltage while Peltier heat is absent at this voltage, a phenomenon explained by examining the energy band diagrams of the layers at these voltages.

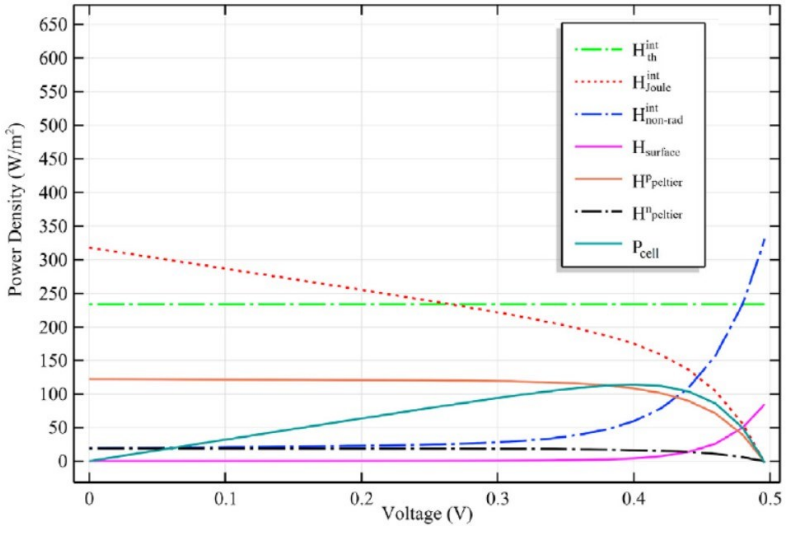

Fig. 1, The power density of all heat generation factors versus voltage

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Development of automated high-throughput modules for accelerated discovery of new battery materials

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Abstract

Over the recent decades, the energy storage demand has dramatically increased as its applications continue to take off. Consequently, it is crucial to intensify research efforts in exploring novel systems and chemistries to keep up with the accelerated demands [1].

This research presented here relies on developing new electroactive materials. This challenge requires rethinking approaches that allow rethinking the traditional experimentation process (based on researcher's chemical intuition and trial-error scheme), which is inherently slow and economically expensive, and remains a bottleneck in the process of discovering new materials. [2]

Considerable efforts have been made to integrate new theoretical approaches for efficient identification of potential candidates [3-4] . Despite the increasing recognition of automated high-throughput methods [5-7], there is still ample room for improving the automating systems of battery applications.

To accelerate the exploration of broad chemical spaces, our group is developing an autonomous Materials Acceleration Platform (MAP) to accelerate the exploration rate of new chemical systems for battery applications in a quicker, cheaper, and more reproducible way. This requires a mind change in our approach to materials research, but also building new lab infrastructures and analytical tools, which include automated high-throughput synthesis modules, automated data analysis programs able to handle large amounts of data, as well as AI-aided experimental planners.

In this presentation, we will present several strategies explored at CIC energiGUNE to speed up the different stages of the development of new materials for Li-ion and Na-ion batteries. Such approaches include:

(i) the use of automated machine-learning-aided screenings of materials databases in search for new families of compounds that can be converted into electroactive materials [3];

(ii) the development of modules to automatize inorganic syntheses (e.g. co-precipitation, solvothermal, sol-gel) and characterization techniques (e.g. XRD, electrochemistry);

(iii) the development of analysis tools for automated data treatment and analysis, including a Machine-Learning experimental planner, chemometrics approaches for data analysis of large XAS data sets [8], or the new FullProfAPP that enables automated Rietveld refinements of large series of data, in particular those generated from operando experiments.[9]

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Solar cell performance characterization through combinatorial deposition and automatized I-V measurements and analysis

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Abstract

This work reports on the combinatorial deposition and high throughput characterization of heterojunctions consisting of sprayed, n-type Ga_2O_3 layers, deposited using ultrasonic spray pyrolysis at high temperature from water-based solution, combined with p-type Cu_2O counterpart, deposited by reactive, direct current (DC) magnetron sputtering. After a comprehensive investigation of the properties of the single layers composing the heterojunctions, devices deposited on ITO (indium tin oxide)-coated glass were characterized. They showed high rectification, with open circuit voltage in excess of 900 mV under simulated solar illumination. This demonstrates the favorable band alignment between the sprayed Ga_2O_3 and Cu_2O, with small conduction band offset. The dependence of the electrical transport properties of the heterojunctions on the Ga_2O_3 thickness was probed by the spray deposition of a thickness gradient over a 7.5×2.5 cm substrate area. Over this area, more than 150 solar cells were formed and measured in terms of their dark and illuminated current-voltage characteristics, as well as analyzed, with an automatized hardware and software setup. The solar cell performance was correlated to the Ga_2O_3 thickness. The latter was probed using an automatized approach, based on the measured and Monte-Carlo-simulated EDS spectra, as well as with the structural and optical characteristics of the layers, similarly acquired using laterally resolved X-Ray diffraction and Fourier transform optical spectroscopy measurements.

Automated defect detection workflow using scanning electron microscope and machine learning algorithm: development towards self-driven materials design and innovation.

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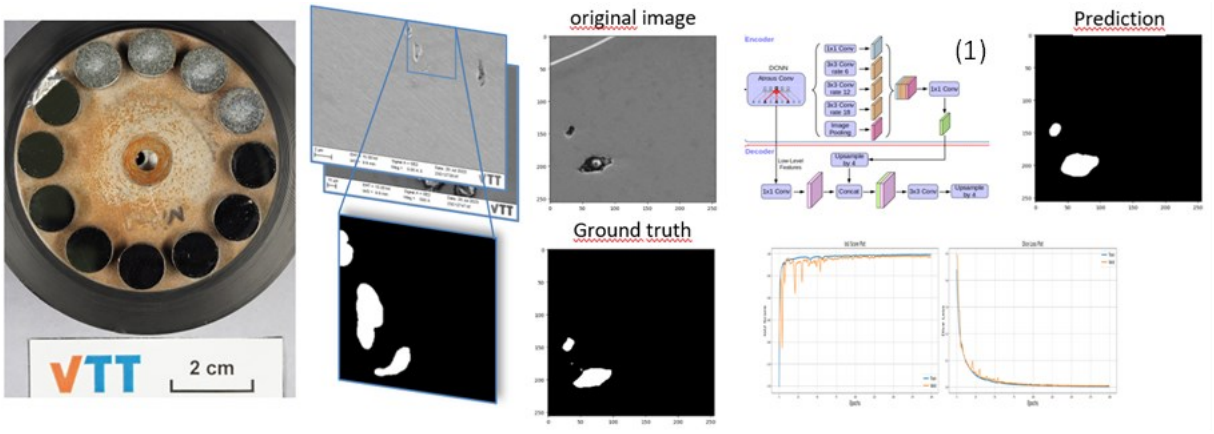
Abstract

Using automated image acquisition and an open machine learning (ML) model to identify various metallurgical defects, we obtained a trained ML model which can detect additively manufactured defects in AISI 316L stainless steel. We printed 12 buttons made of AISI 316L stainless steel as a carousel using direct energy deposition technique. This revolver shaped 12-pin carousel was metallurgically polished using Tegramin automated polishing unit. We observed the microstructural features at 250 randomly chosen region of interests of each button using scanning electron microscope. We used Labkit ImageJ v2 plugin and a macro script-guided semi-automatic image annotation. Thus, we annotated and segmented selected, multiple (>150) images – of resolution 1024 × 768 – to classify background (black = 0) and defects like voids and keyholes (white = 1). We cropped these images into 256 × 256 resolution images for training the ML model based on semantic segmentation. We adopted the DeepLab-v3+ encoder-decoder architecture in this study. We chose intersection over union (IoU) and dice loss (DL) as two measurable parameters for goodness of fit. Our test data mean IoU score is 0.9452 and mean DL is 0.0389 after using 200 epochs on Adam optimizer. In this work we will demonstrate the progress and outlook towards automated characterization to develop materials acceleration platform for future materials design and performance evaluation.



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Bayesian Optimization with Experience for Fast Development of Monolithic Tandem Solar Cells: Simulation Case Study

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Abstract

Machine learning (ML) is gaining more attention in photovoltaic research and will be a vital tool in reaching record-high power conversion efficiencies (PCE) in the near future. One area where ML is significantly beneficial is reducing the number of experiments needed to find the optimum combination of parameters in solar cell fabrication. Bayesian optimization (BO) provides routes for quickly identifying optimum parameters in problems with large parameter space. In this work, we demonstrate that the BO algorithm with experience built with rank-weighted Gaussian process ensemble (RGPE) [1] results in faster optimization of tandem solar cells, a technology rapidly gaining more interest due to its potential to deliver record-high performance. Namely, we show that in the space of 5×10^7 possible parameter combinations, optimum PCE can be obtained after 2 batches/iterations (10 parameter combinations per batch) of experiments/simulations. Moreover, we demonstrate that RGPE method outperforms method without experience (STD) by yielding an increase of ~9%$_{abs.}$ (compared to only 2%$_{abs.}$) in the 2nd iteration and requiring 5× less time to reach a target PCE of 38.5% across 20 different trials (shown in Figure). Results from this work help accelerate the development of tandem solar cells by removing the need for large numbers of experiments in identifying optimum parameters.

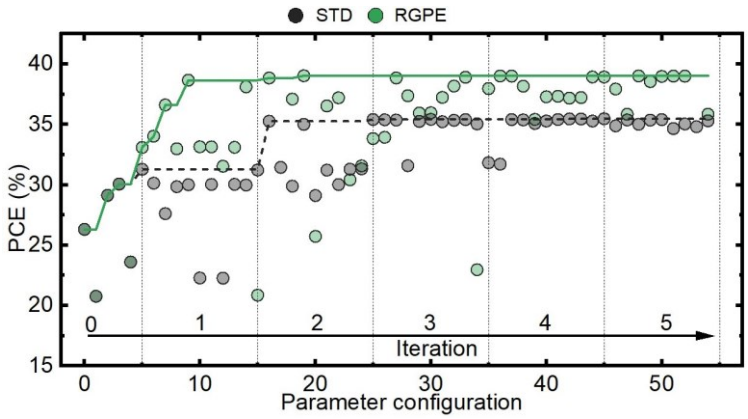

Figure: Exemplary optimization progress of tandem solar cell's PCE using BO methods in this work. Circles represent obtained PCE within a batch. Lines show the maximum obtained PCE.

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Accelerating the Design and Integration of Electrocatalyst Materials for Hydrogen Technologies with Theory and Computation

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Abstract

The discovery of highly performing and durable electrocatalyst materials and the optimal design of electrocatalytic media are crucial enablers of renewable hydrogen technologies, including water electrolysers and fuel cells. In this realm, we develop and use scale-bridging approaches in theory and modelling to track the impact of modifications at the materials level, including electrocatalysts or ionic polymers, on effective properties and performance at the device level. A central theme of our activities is to study the fundamental properties of electrochemical interfaces as a function of their atomistic composition and structure. Through these efforts we gain access to the local reaction environment (LRE) under which desired reactions, e.g., oxygen evolution or CO_2 reduction, as well as undesired processes, such as catalyst dissolution or particle loss, occur. Combining interface models with multiscale and multicomponent transport models allows rationalizing the distribution of reaction rates (DRR) and the overall electrocatalytic performance of porous composite electrodes. Once implemented successfully, the modeling workflow can yield sophisticated materials assessment tools, e.g., multiparametric activity-stability descriptors. Suitable descriptors should – in a highly condensed way – account for intrinsic, structure-based and composition-related properties and represent local conditions (such as the LRE) and distributed properties of materials (such as the DRR). Moreover, they should exhibit a high correlation to device level metrics of performance, lifetime and economic viability. The presentation will highlight major challenges along this path and accentuate opportunities for theory and computation, connected and coordinated with AI-based methodologies in data analytics and machine learning, to accelerate the path from materials discovery to device-level integration.

Machine learning assisted development of metallic hydrides

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Abstract

Machine learning (ML) is increasingly being applied in the development of metallic hydrides for hydrogen storage, a vital component in the advancement of clean energy technologies. The application of ML in this field primarily focuses on the discovery and optimization of new hydride materials that can efficiently and safely store hydrogen with minimum energy losses.

This study focuses on advancing machine learning models to accurately predict the standard equilibrium pressure during hydrogenation, a critical parameter in identifying suitable materials for specific hydrogen use cases. Building upon the foundational models established at Sandia National Laboratories [1], this work represents a significant enhancement, offering more precise predictions and contributing to the optimization of hydrogen storage solutions.

Several machine learning algorithms such as Random Forests and Support Vector Machines from the Scikit-learn library have been applied to a dataset containing both experimental and calculated thermophysical data on metal hydrides compiled as part of a collaborative effort between University of Turin and Sandia National Laboratories.

Furthermore, a recently proposed data augmentation method called PAirwise Difference Regression (PADRE) [2] has been applied to the dataset, significantly increasing the number of items in the dataset. The effectiveness of data augmentation is analyzed and the results are compared with those obtained from enlarging the dataset with new experimental data.

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Materials properties extraction with interpretable artificial intelligence

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Abstract

Material properties extraction has been accelerated during the past decade, with artificial intelligence (AI) and machine learning (ML) techniques leading the way towards novel prediction and analysis methods. Existing and newly generated material properties databases are employed to extract hidden patters from data and suggest new computational models to upscale materials simulations to the macroscale with first principles accuracy. As a first step, property extraction with statistical ML has been incorporated to address the obvious need to take advantage of the available data and follow a shorter path to explain materials behavior. Therefore, “black-box” models have been applied, with predictions that could either interpolate or extrapolate over a given parameter space. Nevertheless, to move beyond this classical approach, explainable, interpretable, generalizable and transparent AI has emerged. One of the techniques capable of providing mathematical expressions that describe a specific material’s behavior with appropriate system variables, is symbolic regression (SR). Differentiating itself from conventional regression methods (e.g., linear, polynomial, etc.), SR spot important features for a physical problem and constructs an analytical equation[1]. Our group has successfully applied SR to extract symbolic expressions even when no theoretical equation was available, such as thermal conductivity and viscosity in simple fluids[2], electrical conductivity of ionic liquids[3], as well as flow rates in rarefied flows[4]. We now focus on the construction of general framework, that will spot all parameters that affect the properties of a material and provide a meaningful expression that can be explained in terms of physical consistency, bypassing costly experiments and/or simulations, where possible.

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Characterization of impurity contamination in solar cells with the assistance of machine learning

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Abstract

Research related to sustainable clean energy technology and artificial intelligence is currently one of the most intriguing areas of interest. Publications at the intersection of these two crucial directions are also emerging. For example, machine learning techniques are utilized for solar cells (SCs) design and for the prediction of material properties essential to their production. Our work focuses on developing the physical foundations of a method aimed at assessing impurity concentrations in solar cells, based on applying machine learning to data obtained from current-voltage characteristics measurements. Such a method is express, low-cost, and does not require additional equipment, making it significant for material engineering applications.

The capability of this method is demonstrated by its application to monocrystalline silicon SC, which make up about 90% of worldwide photovoltaic production capacity, and iron atoms - ubiquitous yet efficiency-reducing impurities. Input features used to determine iron concentration N_{Fe} included SC parameters (base depth and doping level) and changes in photoelectric parameters (short-circuit current, open-circuit voltage, efficiency, and fill factor) after the decay of iron-boron pairs. The machine learning methods included artificial deep neural networks (DNN) and random forest (RF). The training and test datasets were generated by SC simulation performed using SCAPS-1D software over a temperature range of 290-340 K, under AM1.5 and monochromatic light (940 nm) illumination conditions. The hyperparameters of DNN and RF were optimized through a thorough tuning process. The predictive capabilities of deep neural networks and random forests for iron concentration prediction (range of 10^{10}-10^{14} cm^{-3}) were explored, depending on the number of input features used. It has been observed that the mean squared error for the test set could be down to 2 10^{-3}, and random forest predictions were less accurate—see Fig.

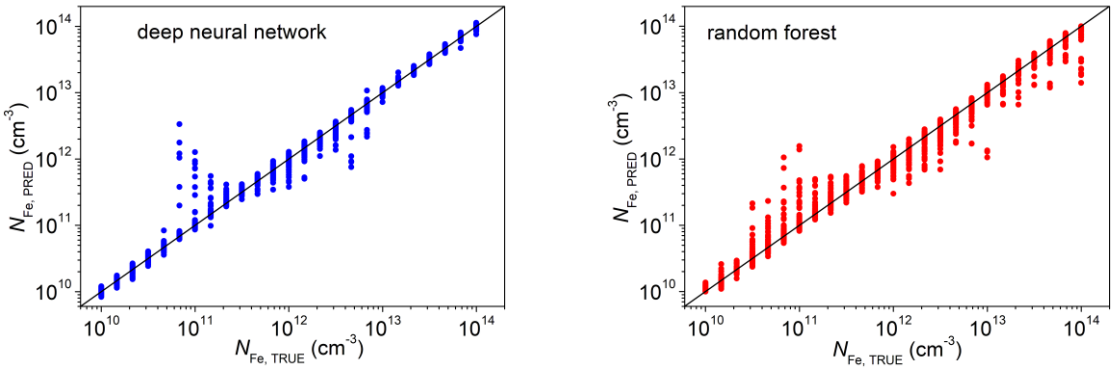

Fig. The prediction results of the DNN (left panel) and RF (right panel) for the test dataset, obtained for AM1.5 illumination condition. The black lines are the identify lines servings as the references

Advanced materials for hydrogen liquefaction and transportation

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Abstract

Hydrogen is considered as the all-round solution for simultaneously combining greenhouse gases emission reduction with uncostly, efficient, and sustainable energy storage and transport [1]. One of the concerns confronted when tackling the latter issue is how to effectively liquify gaseous hydrogen from the deposits inside which it will be stored. In recent years, magnetic shape memory alloys, advanced materials of the ternary Heusler family, have emerged as potential active agents capable of driving an efficient and economically viable cryogenic refrigeration cycle based on the magnetocaloric effect [2] (Figure 1). Complementarily, they can convert the degraded thermal energy generated in the process into useful energy, thanks to the significant magnetization variation associated with thermally-driven phase transitions [3]. In this contribution, a scientific case is provided, which showcases empirical and computational combinatorial screening procedures aimed at finding the most promising alloys and the concomitant necessary dopants compatible with the maximum number of practical requirements. The challenge lies in improving thermal energy transport while simultaneously maximizing magnetisation jumps and minimising thermal hysteresis losses, both keeping in mind safe and sustainable by design (SSbD) approaches in compliance with FAIR principles as well as eventual applications of digitally driven manufacturing and automation techniques.

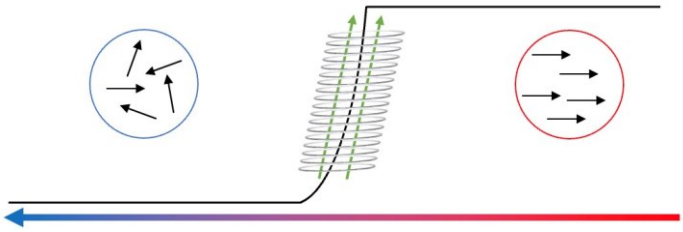

Figure 1. Sketch showing the heat-magnetisation relationship.

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Toward the Italian Energy Materials Acceleration Platform: database implementation with perovskite oxide materials for electrolyzers

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Abstract

Materials Acceleration Platforms (MAPs) can revolutionize the field of perovskite oxide-based CO_2 electroreduction catalysts by accelerating the discovery of new materials and correlations, exploiting the integrated use of experiments, modeling and artificial intelligence (AI). AI algorithms can analyze large experimental datasets to identify relationships between material properties and CO_2 electroreduction activity, guiding the design of materials with improved performance. Additionally, AI can optimize perovskite oxide synthesis, leading to more efficient and cost-effective synthesis methods. This information will be used in the Italian Energy Materials Acceleration Platform (IEMAP) to design new materials with improved performance for the CO_2 electroreduction in Solid Oxide Electrolysis Cells (SOECs). Aiming at both data-driven materials discovery and materials synthesis optimization, herein some experimentally-driven correlations between synthesis, structure and properties are described, along with possible machine learning approaches. Doped $LaFeO_3$ perovskite oxides with different composition were prepared by two different chemical methodologies (solution combustion synthesis, sol-gel Method) and characterized by X-ray diffraction combined with Rietveld refinement, temperature programmed reduction experiments and electrochemical impedance spectroscopy. The obtained results were examined, and some measurable values were selected to fill the IEMAP excel data sheet, giving a concrete contribute to the IEMAP database. This information can be useful to find new correlations between material properties and CO_2 electroreduction activity and can lead to the development of more efficient and cost-effective synthesis methods, which is essential for large-scale production of materials.

Acknowledgements

The Project “Italian Energy Materials Acceleration Platform” (IEMAP) – CUP B82C21001820001 in the Program Mission Innovation is acknowledged for financial support. ISMN authors thank the technicians Francesco Giordano and Nunzio Gallì for their support in the XRD measurement and electrochemical measurements, respectively.

Thermal conductivity study of nanocomposite systems made of porous silicon and liquids

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Abstract

Composite systems, like “porous matrix filled by liquid,” are widely used for energy mining, storage, and conversion. Such systems are often subject to significant thermal loads during their use. Therefore, understanding the thermal properties of composites materials is crucial to develop new pathways for efficient thermal management. On the other hand, ionic liquids are promising for their application as electrolytes for electric battery applications. Due to the continuous miniaturization of the various components of the novel energy storage units, understanding the properties of such liquids under confinement is of prime interest. From this point of view, porous silicon is remarkable as a testing porous material as it allows the possibility to tune the morphology of porous network in a wide range. Therefore, we investigate the thermal transport properties of a nanocomposite systems which is “porous silicon/ionic liquids.” In this framework, first, the heat capacity values of two imidazolium and one ammonium ionic liquids were determined using the method of differential scanning calorimetry, and the thermal conductivity was determined by the photoacoustic approach in the piezoelectric configuration. For the system "porous silicon matrix with the addition of liquid" a photoacoustic approach in the gas-microphone configuration was used to study heat transport properties [1].

Then, the thermal transport properties of a nanocomposite system consisting of porous silicon filled with an ionic liquid were studied. Experimental results shown significant thermal conductivity enhancement compared to the one predicted by effective medium approximation. The composite system exhibited a thermal conductivity more than twice the one of the original porous silicon and more than eight times the thermal conductivity of the ionic liquid alone. These findings have promising implications for heat management and developing high-efficiency energy storage devices.

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NOVEL IDEAS IN PRECONDITIONING ITERATIVE SOLVERS FOR PDEs SOLVING

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Abstract

Materials science as so many other scientific areas demands the efficient solving of systems of Partial Differential Equations (PDEs), then research in better numerical methods is a must. Solvers involved in this task typically deal with a huge number of degrees of freedom (DoFs). And DoFs become extremely large when multiscale modelling is in the simulation paradigm: besides a PDEs system there is a meso/micro-scale approach to modelling, tackled in a coupled manner. Thus time-to-solution becomes crucial to find accurate enough solutions in a reasonable time.

Many exciting issues are part of this endeavour: exascale stencils, parallelization, time integration, direct solving, iterative solving, acceleration techniques (preconditioning and others),... Among then this talk will focus on the especific issue of preconditioning systems of equations due to it is a workhorse in the design of efficient iterative solvers.

At present our group is involved in the development and implementation of a novel, parallel preconditioner based on the randomized Singular Value Decomposition (SVD) algorithm, tested with a Krylov subspace GMRES solver. This work is being advanced in two fronts: serial developments for prototyping and testing of ideas; and parallel implementation for benchmarking of performance, which is done using the well-known PETSc framework with the plugin SLEPc (developed at the Polytechnic University of Valencia, Spain) which extends its functionality to parallel SVDs objects. The mentioned benchmarking is conducted over a large enough set of problems, which provide a rich variety in terms of spectral content. A key idea of this formulation is to exploit the typically found low-rank behaviour of an error matrix which arise after the ILU(0) factorization. Interestingly, this low-rank property leads to bound the computing-cost of the randomized SVD factorization, then a more efficient preconditioner can be applied during the Krylov iteration. The attained benefit in shortening the iterations-to-solution is promissing, and the extra flops needed to build the mathematical entities required by this approach will be discussed. Some recent results illustrating its performance will be shown.

Integrating Experimental and Computational Techniques for Enhanced Characterization of Material Properties: A Focus on Dislocation Densities and Residual Stresses

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Abstract

The endeavor to comprehensively understand and predict the behavior of materials under various conditions necessitates the integration of experimental data with computational models—a process known as coupling characterization. This multidisciplinary approach bridges the gap between empirical observations and theoretical simulations, allowing for the enhanced fidelity of material models and predictions. Specifically, the characterization of dislocation densities and residual stresses represents a critical aspect of this process.

Dislocation densities, which are quantifiable imperfections within the crystalline structure of materials, are pivotal in determining mechanical properties such as yield strength and ductility. Experimental techniques such as electron backscatter diffraction (EBSD) provide a means to measure these dislocations directly within the microstructure. On the other hand, computational methods like discrete dislocation dynamics (DDD) simulations offer predictive insights on how dislocation densities evolve under various loading conditions.

Residual stresses, the stresses that remain in a material after the original cause of the stress has been removed, significantly affect material performance and structural integrity. Experimental techniques to measure these stresses include X-ray diffraction (XRD) and neutron diffraction, which can provide non-destructive evaluation of stress distributions. The methods such as finite element analysis (FEA) can simulate stress states in complex geometries and loading conditions.

The coupling of these characterization methods entails the calibration of simulation parameters using experimental data, enhancing the predictive capability of computational models. The advances in coupling characterization not only enhance the understanding of material behavior but also expedite the development of novel materials with tailored properties, optimizing performance for specific applications. This integration of experimentation and simulation is a cornerstone of modern material science, pushing the boundaries of innovation in material design and engineering.

An equivalent circuit model-based analysis for the energy conversion chain from PV source with a supercapacitor as DC-link

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Abstract

In the realm of new energy materials and devices, efficiently interfacing electricity-generating devices with storage devices and specific loads is often overlooked. While individual device optimization is common, the overall system's synergetic performance is frequently neglected. In order to develope highly efficient energy systems, electricity conversion interfaces, particularly DC/DC links and converters, are becoming increasingly crucial. In this work, a comprehensive circuit model-based analysis of PV source to constant power load conversion chain, in which a supercapacitor (SC) is used as DC-link, is presented. Due to the intermittent and random nature of the PV source it is always necessary to regulate its voltage and current to ensure that the electrical and electronic loads for which this energy is generated are duly powered. The main problem related to power supply from a PV source is due to the double need to adapt the voltage to the load, but at the same time ensure that the source operates at its maximum power point (MPPT techniques). For this reason, it is necessary to use two DC-DC converters to obtain a double degree of freedom. The supercapacitor is inserted as a DC-link between the two converters, to decouple them, stabilize the voltage and as a storage element. Supercapacitors have many advantages over traditional batteries; however, they have a voltage behavior dependent on the state of charge like classic capacitors. Therefore, we propose a model in which the conversion chain is divided into multiple individually modeled blocks, thus allowing to derive the voltage profile on the supercapacitor and adjust the voltage and current gains of the DC-DC converters to avoid unstable conditions. The proposed modular modelling methodology allows the investigation to be performed with different storage, generation and conversion blocks according to the necessity of the application under study. Moreover, it can serve as a benchmark to study control techniques for MPPT in dynamic and partial shading conditions, control of the DC-DC stages for maximum efficiency, and smart management of the storage to reduce degradation.

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A New Class of Descriptors for Nanoporous Materials and its Applications to Classification and CO2 Gas Adsorption int zeolites

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Abstract

The generalization of the high-throughput synthesis has recently allowed the discovery of thousands of new porous materials generating a large amount of information with the development of specialized databases. Widespread access to databases enabled the increase of algorithms and models for property prediction and in-silico design of materials. The structural information of materials still needs to be rationalized by the inclusion of descriptors to ease the characterization of solids. This is essential for in-silico screening to potential applications based on Machine Learning (ML) approaches. Indeed, at the forefront of a real revolution in the selection and design of porous materials for many industrial applications, the use of appropriate descriptors to encode solid material properties (topology, porosity, surface chemistry) is one of the fundamental aspects in the development of ML-based models. Our analysis of the literature reveals a lack of descriptors based on the Potential Energy Surface (PES) of crystalline materials embedding crucial information such as the porosity, the topology, and the surface chemistry. In this work, we introduce new PES-based descriptors including the surface probability distribution of the local pore curvature (K_H), the electrostatic-potential energy surface distribution (σ_e), as well as the local electrostatic-potential gradient surface probability distribution ($\nabla\sigma_e$). Our descriptors allow the classification of zeolites (Fig 1.a) as well as its characterization by self-containing standard morphological and topological information (pore diameter, tortuosity, surface chemistry, etc.). We illustrate their usage to generate accurate ML-based models of isosteric heat of adsorption of CO_2 on purely siliceous zeolites of the IZA database (Fig 1.b) and ion-exchanged zeolites in function of the Si/Al ratio for the case of LTA topology.

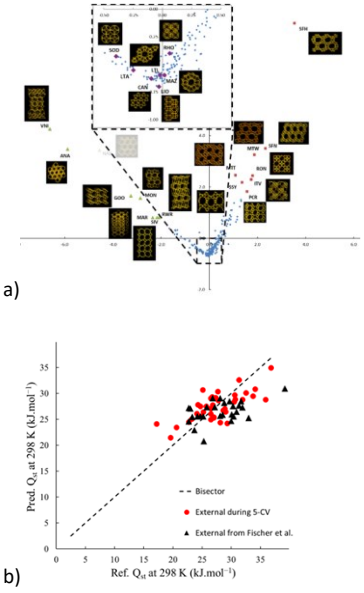

Fig. 1.a V-Shape classification map of the International Zeolite Assoc. (IZA) database. b) Parity plot of isosteric heat of adsorption of CO_2 on IZA zeolites predicted using Support Vector Machine (SVM) and our descriptors