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Context of the research activity	Health, advanced manufacturing, environment, energy. These words describe some of the grand challenges for the next future. We believe that new simulation and virtualization technologies, from large-scale computing to artificial intelligence, have the potential to unravel the complexity posed by these global challenges. The proposed research project targets the design and development of **innovative materials, processes and devices for Industry 4.0** applications through **advanced and high-throughput AI technologies**. In a **strongly interdisciplinary and international environment**, we work in close contact with researchers and institutions from both **academia and industry.** Our headquarters are at the **CNR Research Area in Bologna**, hosting about 800 researchers/technicians, the CNR Technopole, Accelerators of Innovation and Incubators, Technology Transfer Offices and Agencies, and next to the new University of Bologna Campus. Our position, **in the hearth of the European Data Valley** (https://www.ifabfoundation.org/), allows us to interact and cooperate with strategic actors for AI in Industry 4.0, from competence centers for industrial innovation to academic research centers. Our approach allows us to **close the loop from research to innovation** in the context of real-life applications. In addition to hosting a national-level infrastructure for high-performance computing, data science and AI, we collaborate with large-scale national and international supercomputing facilities (CINECA, etc.).

Objectives	The overarching objective of the research project is the **development of a data-driven framework for the design of materials, materials processes and devices for advanced manufacturing**. Starting from the extension of AI and ML/DL technologies to materials science, the project aims at providing a virtual platform for the development of advanced materials and automated production systems. The research project will initially target materials for nanotechnologies, which are key enablers for a wide set of industrial applications (4^{th}-generation photovoltaic solar cells, medical and wearable devices, smart sensors, etc.). Next, the project will address the large-scale manufacturing of engineered materials. The specific targets will be selected on the basis of use-cases emerging from **collaborations with experimental and industrial research groups**.

	The key objectives are the following: • Extension of current technologies for the representation of knowledge and information in the field of advanced materials. • Development of strategies for the integration of simulated and non-simulated data obtained from high-throughput approaches (HPC modelling, sensors, etc.). • Application of ML and generative models for the "inverse design" of new nanomaterials • Development of a data-driven generalized framework for the automatization of manufacturing processes. • Development of new devices and/or technologies based on novel materials and materials processes for specific applications and large-scale automation. To accomplish these objectives, the research work will be carried out in the framework of current activities of the hosting research group and in collaboration with other groups and institutions at the local, national and international level.

Skills and competencies for the development of the activity	**Minimal skills** are: • Good/very good command of Linux OSs • Good general coding skills • Basic knowledge of ML methods • Basics of calculus, data analysis and visualization **Extra skills** include: • Programming skills in Python, Julia, Rust (C, C++, Fortran) • Prior experience in the development of ML and DL frameworks and knowledge of common framework and libraries (scikit-learn, TF, Keras, PyTorch, etc.) • Skills on knowledge representation, formal languages and ontologies • Skills on data warehousing • Skills on parallel computing libraries (MPI, OpenMP) and HPC infrastructures and management • Skills on multiscale simulations for materials science and engineering • Experience on tools for collaboration, visualization and sharing (git repositories, Jupyter notebooks, 2D and 3D graphics, etc.)