POLITECNICO DI MILANO

PhD in FISICA / PHYSICS - 38th cycle

THEMATIC Research Field: DESIGN OF NOVEL MULTIFUNCTIONAL MATERIALS: AB-INITIO SIMULATIONS, HIGH-THROUGHPUT AND MACHINE-LEARNING APPROACHES FOR BULK AND NANO-SCALE MATERIALS

Monthly net income of PhDscholarship (max 36 months)
€ 1400.0 In case of a change of the welfare rates during the three-year period, the amount could be modified.

Context of the research activity	
Motivation and objectives of the research in this field	Materials design is currently undergoing a revolution, driven by the increasing importance of machine learning (ML) approaches as a boost for materials discovery. While at present ML for quantum matter is rather unshaped, it is likely to dramatically develop in the next decade, with all materials¿ classes (including functional compounds such as ferroics) expected to benefit from artificial intelligence. Ferroic materials (magnetic, ferroelectric, etc) are particularly difficult to model on the basis of ¿intuition¿ or simple ¿rules of thumbs¿, due to their inherent complexity. Furthermore, they often present cross-coupling phenomena (magnetostriction, piezoelectricity, magnetoelectricity), which makes them very useful from the application point of view, but at the same time extremely difficult to predict and optimize without a complex theoretical machinery. The combination of first-principles simulations based on density functional theory (DFT) and of ML approaches represents therefore a powerful tool for future materials design.
Methods and techniques that will be developed and used to carry out the research	The research activity will involve developing a code for ML oriented towards the detailed understanding of microscopic mechanisms underlying materials¿ functionalities and towards design of functional compounds with optimized properties of technological relevance for microelectronics. The code, aimed at identifying via ML complex descriptors characterizing the property of interest, will be tested starting from different

	DFT databases present in the literature for functional materials, possibly incremented, for a better accuracy, via high-throughput DFT simulations performed by the candidate. The work will be carried out jointly at Politecnico di Milano, Consiglio Nazionale delle Ricerche CNR-SPIN in Chieti and STMicroelectronics.
Educational objectives	Development of interdisciplinary knowledge at the boundary between computational materials science, machine learning and applied physics.
Job opportunities	While the competences developed during the PhD will mostly be related to computational materials science and ML, the activity will be carried out in close contact with experimental groups at Politecnico di Milano and with industrial research groups at STMicroelectronics. This inherent multidisciplinarity will grant possibilities for careers both in academia and in industry.
Composition of the research group	1 Full Professors 2 Associated Professors 2 Assistant Professors 4 PhD Students
Name of the research directors	Silvia Picozza, Laura Castoldi, Riccardo Bertacco

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Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents (more than 80Km out of Milano)	--

Scholarship Increase for a period abroad	
Amount monthly	700.0 €
By number of months	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information

Educational activities:

Educational activities (purchase of study books and material, funding for participation to courses, summer schools, workshops and conferences): financial aid per PhD student per 3 years: max 5.707,13 euros per student.

T**eaching assistantship:**
There are various forms of financial aid for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities, within the limits allowed by the regulations.

Computer availability: individual use
Desk availability: individual use