PhD in INGEGNERIA DEI MATERIALI / MATERIALS ENGINEERING - 41st cycle

BORSE TEF Research Field: EXPLOITING QUANTUM COMPUTING FOR QUANTUM CRYSTALLOGRAPHY

Monthly net income of PhDscholarship (max 36 months)
1800.0 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	The ability to derive wave functions directly from experimental data represents an exciting and intellectually stimulating challenge, which has attracted the attention of several research groups over the years. At the heart of this endeavor lies the search for a physically meaningful entity capable of encapsulating all the information gleaned from an experiment. According to the principles of quantum mechanics, the wave function stands out as the most appropriate candidate for this purpose. Within this framework, the X-ray restrained wave function (XRW) method introduced by Jayatilaka is arguably one of the most significant advancements. Building on the earlier ideas of Henderson and Zimmerman and on the constrained search formulation of density functional theory (DFT), the Jayatilaka approach represents the first viable strategy of quantum crystallography for obtaining accurate single Slater determinant wave functions that not only adhere to the principles of quantum mechanics but that also reproduce experimentally observed diffraction intensities. The objective of this project is to substantially enhance the above mentioned XRW methodology by integrating it with emerging quantum computing technologies. By leveraging the considerable advantages offered by quantum computation, the goal is to develop a more refined and powerful multi-determinant XRW approach

	based on the Unitary Coupled Cluster (UCC) wave function ansatz. The resulting “experimental wave functions” are expected to offer unprecedented insights into the properties of molecules and solids, thus representing a new possible powerful tool for theoretical studies aimed at designing novel materials.
Methods and techniques that will be developed and used to carry out the research	The aim of this PhD project is to develop a quantum computing version of the X-ray Restrained Wave Function (XRW) method. This advancement will pave the way for the first truly multi-determinant XRW technique, leveraging the variational nature of the Unitary Coupled Cluster (UCC) wave function ansatz. The research will be structured into three main phases: **Phase 1 - Literature Review and Experimental Data Acquisition** In the initial phase, the PhD candidate will focus on acquiring a comprehensive understanding of both the XRW methodology and quantum computing, with particular attention to its applications in quantum chemistry. This will involve an in-depth review of the relevant literature, which will be regularly discussed with the project supervisor. Simultaneously, experimental data will be gathered, primarily through high-resolution X-ray diffraction measurements conducted at the Politecnico di Milano. **Phase 2 – Method Development and Quantum Algorithm Implementation** The second phase will involve the theoretical development of the new approach, beginning with the derivation of the fundamental equations required to formulate the quantum algorithm. The initial design and implementation will take place at the Politecnico di Milano under the guidance of the project coordinator. Subsequently, the algorithm will be further refined in collaboration with the Laboratoire de Chimie Quantique at the Université de Strasbourg (France), in close partnership with CNRS researcher Dr. Saad Yalouz (LCQ Strasbourg – Saad Yalouz). During this stage, the algorithm will be rigorously tested and validated against both experimental data and theoretical benchmarks.

	Phase 3 – Dissemination and Application of Results In the final phase, the focus will shift to the continuous refinement and application of the quantum algorithm. The method will be applied to a diverse range of systems to demonstrate its accuracy, efficiency, and practical utility. The outcomes (both in terms of methodological innovation and scientific applications) will be disseminated through peer-reviewed publications and other academic channels.
Educational objectives	The primary objective is to prepare the PhD student as a wellrounded researcher, equipped to pursue a career in both academic and non-academic sectors. The project also aims to introduce the student to the cutting-edge fields of quantum computing and quantum crystallography at a practical level.
Job opportunities	Recent PhD graduates in quantum computing and quantum crystallography have access to a growing range of professional opportunities across academia, industry, and government sectors, due to the increasing global investment in quantum technologies.
Composition of the research group	2 Full Professors 4 Associated Professors 8 Assistant Professors 7 PhD Students
Name of the research directors	Prof. Alessandro Genoni

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Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents	--

Scholarship Increase for a period abroad	
Amount monthly	900.0 €
By number of months	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
Confidentiality: since this is a thematic scholarship, the management of Confidential Information, Results and their publication should be subordinated to restrictions. Upon acceptance of the scholarship, the beneficiary may sign a specific commitment. **Educational activities** (funding for participation in courses, summer schools, workshops and conferences) - financial aid per PhD student per year: 1st year: around 2,400 euros 2nd year: around 2,400 euros 3rd year: around 2,400 euros **Teaching assistantship**: availability of funding in recognition of supporting teaching activities by the PhD student. There are various forms of financial support for activities of teaching practice. The PhD student is encouraged to take part in these activities within the limits allowed by the regulation.