POLITECNICO DI MILANO

PhD in INGEGNERIA DEI MATERIALI / MATERIALS ENGINEERING - 39th cycle

PARTENARIATO PNRR Research Field: QUANTUM COMPUTING SOFTWARE FOR QUANTUM CHEMISTRY AND CRYSTALLOGRAPHY

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	PNRR CN HPC big data e quantum computing CUP D43C22001240001 Spoke 10 Decreto di concessione: n. 3138 del 16/12/ 2021 It is well established that quantum computing (QC) will affect disruptively many areas of science and technology. Among the expected applications, quantum chemistry is one of the least explored so far, despite the predicted benefits of this revolutionary technique for the purposes of computational chemistry. The molecular electronic structure problem is at the core of computational chemistry. This means solving the Schrödinger equation for the ground and low-lying electronic states of molecules and crystals, the geometries of which may be far away from the minima on their corresponding potential energy surfaces. The current "chemical accuracy", i.e. the ability to predict molecular and crystal structures and their relative energies, is today quite high. For example, errors on relative energies can be smaller than 1 kcal/mol, which is important for modelling chemical reactions, predicting most stable isomers, conformers and polymorphs. However, as the size of the system grows, the computational costs also increase and more severe approximations must be applied, which reduces significantly the chemical accuracy of the calculations. This mainly affects the possibility to include sufficiently the electron correlation into the calculated wavefunctions and

	therefore be unable to correctly predict particular states (especially transition states, excited states, etc.). The aim of this project is testing the feasibility of quantum computing to obtain more accurate molecular and crystal geometries, as well as energies and wavefunctions. We will adopt methods capable of describing electron correlation in molecules and solids, which could also include information from experimental observations such as X-ray diffraction intensities.The research is funded through the national center for high performance computing, big data, and quantum computing. https://www.supercomputing-icsc.it/en/icsc-home/The research will be carried out at the Laboratory for Materials Modelling, Morphology and Structure of the Department of Chemistry, Materials, and Chemical Engineering of the Polytechnic of MilanMore information about the research is available athttps://3most.chem.polimi.it/quantum-crystallography/
Methods and techniques that will be developed and used to carry out the research	The main methods adopted will be quantum chemical methods, especially post Hartree-Fock techniques that progressively include electron correlation into the wavefunction. Among these, we will test spin-coupled techniques, able to include in a single determinant wavefunction the largest part of the electron correlation. As for the quantum crystallographic tools, we will use X-ray restrained wavefunction techniques.Data programming will be developed within QC platforms, such as qiskit.
Educational objectives	The PhD will gain new knowledge on: a) QC programming; b) QC applications to quantum chemical problems; c) implementation of QC software on quantum computers.
Job opportunities	The rapidly growing field of quantum computing let us envisage excellent opportunities for students who undertake now a PhD project and that would graduate in three-year time. The specific applications of quantum computing for quantum chemical problems is also very innovative and it is expected that a PhD graduated with such an expertise will easily find academic post-doc

	research positions, once completed the PhD course.
Composition of the research group	3 Full Professors 3 Associated Professors 0 Assistant Professors 3 PhD Students
Name of the research directors	Prof. Piero Macchi; Prof. Antonino Famulari

Contacts
piero.macchi@polimi.it https://3most.chem.polimi.it/

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

The candidate will have to fill in a mandatory questionnaire in order to close the application.

Individual budget for research (5.700 euro):1st year: 1.900 euro; 2nd year: 1.900 euro; 3rd year: 1.900 euro

Teaching assistantship: availability of funding in recognition of supporting teaching activities by the PhD student. There are various forms of financial of 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 regulation.