Topic title	High quality and hardware-efficient wavefunctions for quantum molecular dimulations
Main host institution	University of L'Aquila, Italy https://www.univaq.it/en/
Supervisor	Leonardo Guidoni, University of L'Aquila, Italy leonardo.guidoni@univaq.it
Co-Supervisor	Ivano Tavernelli, IBM Research, Switzerland ITA@zurich.ibm.com
Mentor[1]	Daniele Ottaviani, CINECA (Bologna), Italy d.ottaviani@cineca.it
Secondment institutions	IBM Reseach, Switzerland (5 Months) and CINECA, Italy (1 Month)
Preferred starting date	1st of October 2021

Topic description

The project deals with the development of new strategies to tackle the electronic structure of molecular systems using quantum computers. The use of Noisy Intermediate-Scale Quantum (NISQ) devices in combination with algorithms such as the Variational Quantum Eigensolver are a valuable route to reach the chemical accuracy of the evaluation of ground state molecular energies. A crucial role in this process is to design wavefunctions that are at the same time accurate and compact, in order to have low-dept circuits using a small number of gate operations. The student will develop hardware efficient wavefunctions and algorithms inspired by many-body and quantum chemistry techniques. Error mitigation schemes will be also developed to further increase the accuracy of the obtained results. The developed methodology will be applied to several chemical systems, including well-known correlated and "difficult" cases in quantum chemistry.

Recommended applicant's profile

Candidates should hold a Master Degree in Physics or Chemistry with a strong background in quantum mechanics and molecular simulations. Good skills in computer programming are also recommended.

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[1] Mentor: The primary role of the mentors will be to identify and facilitate specific training objectives, advise on any problems faced by the ESR, including career matters with an external perspective and provide mediation in the case of disputes.