

Topic title	Simulation of electronic structure properties in near term quantum devices
Main host institution	IBM Quantum, IBM Research Zurich, Switzerland https://www.zurich.ibm.com
Supervisor	Prof. Dr. Ivano Tavernelli ITA@zurich.ibm.com
Co-Supervisor	Prof. Dr. Frank Wilhelm-Mauch, Saarland University/FZJ, Germany f.wilhelm-mauch@fz-juelich.de
Mentor¹	Prof. Dr. Guido Pupillo, Strasbourg University, France pupillo@unistra.fr
Secondment institutions	Saarland University, Germany (4 Months) Universita dell'Aquila, Italy (2 months)
Preferred starting date	Upon agreement, at the latest until October 2021
Topic description	
<p>The accurate solution of the Schrödinger equation using classical algorithm is hampered by the exponential scaling of the problem size. Quantum computers can overcome this limitation thanks to the possibility to encode the exponentially large Hilbert space in a qubit register that scales linearly with the number of electrons. This project will focus on: (i) investigating wavefunction Ansätze for quantum circuits based either on classical algorithms (e.g., Coupled Cluster, CASSCF and Quantum Monte Carlo) or purely quantum computing solutions (e.g. hardware efficient quantum circuits), (ii) design new strategies to go beyond conventional VQE (e.g. imaginary-time propagation; improved classical optimizers; “in circuit” optimization), (iii) extensions to the calculation of excited states properties, (iv) calculation of forces for molecular dynamics in the ground and excited states, and (v) optimization of circuit depth to make the algorithms applicable on near-term noisy quantum computers.</p>	
Recommended applicant's profile	
<p>We are looking for a candidate with a five-year BSc+MSc degree in physics, quantum chemistry or applied mathematics. The candidate should have a good working knowledge of theoretical, mathematical, or computational quantum physics and/or quantum chemistry and at least some past exposure to quantum computing. An outstanding candidate will also have some background in at least one of the areas of programming (advanced Python), numerical simulation.</p>	

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.