

MOQS – MOlecular Quantum Simulations

Topic title	Hardware-optimized state preparation and benchmarking for molecular quantum simulation
Main host institution	Saarland University (in collaboration with Jülich Research Center) https://www.uni-saarland.de / www.fz-juelich.de
Supervisor	Prof. Dr. Frank Wilhelm-Mauch f.wilhelm-mauch@fz-juelich.de
Co-Supervisor	Ivano Tavernelli, IBM Research ITA@zurich.ibm.com
Mentor¹	Prof. Dr. Leonardo Guidoni, University dell'Aquila, Italy leonardo.guidoni@univaq.it
Secondment institutions	Universita dell'aquila, Italy (3 Months) IBM Rüschlikon, Switzerland (3 Months)
Preferred starting date	Flexible within project boundaries – at the latest Oct. 2021
Topic description	
<p>Variational algorithms for chemistry on quantum computers aim at preparing good candidate states for a molecule from fiducial initial states with a quantum protocol parameterized by a number of continuous parameters, which are optimized by an external classical algorithm. In this project, we will look for protocols that, rather than being broken up into a set of quantum gates, use continuous analogue waveforms to accomplish this task in a time-optimal and robust way. We will use algebraic constructions to make sure that the right set of states can be reached and then concepts from quantum optimal control to find hardware-efficient protocols towards that goal. We will collaborate with partner groups to connect to theoretical chemistry as well as to hardware properly. The project will include the opportunity to test results on quantum hardware. The candidate will be integrated into the Wilhelm-Mauch group, which is part of Saarland University and Research Center Jülich. This group offers a rich and stimulating research environment around research in superconducting qubits. Optimal control tools developed in the group are crucial to parts of this research.</p>	
Recommended applicant's profile	
<p>We are looking for a candidate with a five-year BSc+MSc degree in physics - candidates with four-year degrees may also be eligible under some restrictions. The candidate should have good working knowledge of theoretical, mathematical, or computational quantum physics and at least some past exposure to quantum computing or quantum control in a course, a summer school, or a previous research project. An outstanding candidate will also have some background in at least one of the areas of programming, numerical simulation, or Lie group theory – we will teach the rest.</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.