

MOQS – MOLEcular QUANTUM SIMULATIONS

Topic title	Towards simulations of coupled nuclear and electronic dynamics on a quantum computer.
Main host institution	Heidelberg University, Germany https://www.uni-heidelberg.de/en
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Mentor¹	Guido Pupillo, Strasbourg University, France pupillo@unistra.fr
Secondment institutions	IBM Research, Switzerland (3 Months) University of Strasbourg, France (3 Months)
Preferred starting date	01.03.2021 – 01.07.2021 Latest possible start 01.10.2021
Topic description	
<p>In this project, our goal is to develop strategies to represent and solve the coupled nuclear-electronic problem using quantum computers. This involves finding maximally diabatic (slowly changing with respect to nuclear displacements) basis of electronic single particle functions to be used in the q-bit representation of the molecular Hamiltonian. Two routes are envisaged, (1) the quantum computer is used as a co-processor to track the time-dependent electronic wavefunction whereas nuclear dynamics, possibly on the level of classical trajectories, runs on classical hardware. (2) The complete problem is mapped onto a quantum algorithm, with extra qubits representing the motion along nuclear degree(s) of freedom. These developments will be first applied and benchmarked on model systems. Afterwards, we aim at applications where the electronic structure problem involves highly correlated molecular electronic Hamiltonians involving metal complexes with of, e.g., catalytic or biological relevance. For work from our group in a related direction please see [https://aip.scitation.org/doi/10.1063/5.0028116].</p>	
Recommended applicant's profile	
<p>Previous experience (Bachelor/Master) in either <i>quantum (wavepacket) molecular dynamics / electronic structure development or high-end applications / AIMD / quantum algorithms / as well as some programming experience</i> are part of your skill set. You are highly motivated to pursue a PhD in a dynamical and quickly evolving field of research. You enjoy cracking problems, finding creative solutions and thinking out of the box, and you are looking forward to maturing as a young scientist within a team people with similar motivations and inner-drive.</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.