

Università degli Studi di Padova Dipartimento di Scienze Chimiche

Ciclo di Seminari 'Frontiers in Chemistry'

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Quantum Computing and its Applications in Chemistry and Physics

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Quantum computing is emerging as a new paradigm for the solution of a wide class of problems that are not accessible by conventional high performance classical computers. Quantum computers can in principle efficiently solve problems that require exponential resources on classical hardware, even when using the best known classical algorithms. In the last few years, several interesting solutions with potential quantum speedup have been brought forward in the domain of quantum physics, like the quantum phase estimation and the hybrid variational quantum eigensolver for the solution of optimization problems.

The original idea that a quantum computer can potentially solve many-body quantum mechanical problems more efficiently than classical computers is due to R. Feynman who proposed the use of quantum algorithms to investigate the fundamental properties of nature at the quantum scale. In particular, the solution of the problems in electronic structure, material design, high energy physics, and statistical mechanics (just to mention a few) is a challenging computational task as the number of resources needed increases exponentially with the number of degrees of freedom. Thanks to the development of new quantum technologies witnessed over the last decades, we have now the possibility to address these classes of problems with the help quantum computers. To achieve this goal, new quantum algorithms able to best exploit the potential quantum speedup of state-of-the-art noisy quantum hardware have also been developed [1,2]. In this talk, I will first introduce the basics of quantum computing using superconducting qubits, focusing on those aspects that are crucial for the implementation of quantum chemistry and physics algorithms. In the second part, I will highlight the potential advantages of the new generation of quantum algorithms for applications in chemistry [3,4], physics [5] and biology [6].

- [1] N. Moll, et al. Quantum Sci. Technol., 3, 030503 (2018)
- [2] A. Kandala et al., Nature, 549, 242 (2017).
- [3] P. Baroutsos, et al., Phys. Rev. A, 98, 022322 (2018); P. Ollitrault et al., Phys. Rev. Res., 2, 043140 (2020)
 - [4] P. Baroutsos, et al., Chemical Science, accepted (2021); (arXiv:2008.06449).
 - [5] S. Mathis, et al., Phys. Rev. D, 102, 094501 (2020).
 - [6] A. Robert et al., npj Quantum Inf., accepted (2021); (arXiv:1908.02163).

La presenza della S. V. sarà molto gradita.

Prof. Michele Maggini Direttore del Dipartimento di Scienze Chimiche



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