



Lunedì **22 maggio 2023** alle ore **14:30** presso l'aula I

il **Dr. Marco Govoni**

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terrà il seminario dal titolo:

**First principles spectroscopy using
pre-exascale and noisy intermediate-scale
quantum computers**

We present calculations of both the ground and excited states of spin defects in solids carried out on noisy intermediate-scale quantum computers coupled to pre-exascale systems. We focus on point defects, e.g., the NV center in diamond, which are of interest for the realization of quantum technologies. To describe point-defects embedded in periodic crystals we use full configuration interaction embedded in DFT+GW, i.e., we derive an effective Hamiltonian that describes the low-lying excitations of the defect using the quantum defect embedding theory (QDET). We use the variational quantum eigensolver (VQE) and the quantum subspace expansion (QSE) methods to obtain the ground and excited states of spin qubits, respectively, and we propose a strategy for noise mitigation. We show that, by combining zero-noise extrapolation techniques and symmetry-constraining ansätze, one can obtain reasonably accurate results on near-term-noisy architectures for ground- and excited-state properties of spin defects. Finally, we discuss opportunities for electronic structure calculations that are driven by emerging trends in the high-performance computing landscape, which include strategies to leverage exascale and quantum computing.

La presenza della S. V. sarà molto gradita

Stefano Corni

Il Direttore del Dipartimento
Michele Maggini