Università degli Studi di Padova

DiSC

Lunedì **18 settembre 2023** alle ore **14:30** presso l'aula F

il **Dr. Marco Govoni**

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terrà il seminario dal titolo:

Quantum embedding methods to simulate condensed systems on quantum computers

Quantum computers hold promise to improve the efficiency of quantum simulations of materials and to enable the investigation of systems and properties that are more complex than tractable at present on classical architectures. 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 the calculation of photoluminescence from 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 (FCI) 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. We combine a qubit-efficient encoding scheme mapping Slater determinants onto qubits with a modified qubit-coupled cluster ansatz and noise-mitigation techniques. Such strategy leads to a substantial improvement in the scaling of circuit gate counts and in the number of required qubits, and to a decrease in the number of required variational parameters, thus increasing the resilience to noise. Although quantum simulations on quantum architectures are in their infancy, promising results for realistic systems appear to be within reach.

La presenza della S. V. sarà molto gradita

Il Direttore del Dipartimento
Michele Maggini

Stefano Corni