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Simulating condensed systems on quantum computers with quantum embedding

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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. Here, we discuss a computational framework to carry out electronic structure calculations of solids on noisy intermediate-scale quantum computers using embedded Green's function theory [1]. We give examples for a specific class of materials, that is, solid materials hosting spin defects, e.g., the NV center in diamond. These are promising systems to build future quantum technologies, such as quantum sensors and quantum communication devices. The defect is described by an effective Hamiltonian, whose parameters are evaluated from first principles on a pre-exascale computer [2], and whose ground and excited states are obtained using the variational quantum eigensolver (VQE) and the quantum subspace expansion (QSE) method, respectively [3]. Although quantum simulations on quantum architectures are in their infancy, we show that promising results for realistic systems appear to be within reach combining zero-noise extrapolation techniques and symmetry-constraining ansätze [4].

[1] N. Sheng, C. Vorwerk, M. Govoni, G. Galli, J. Chem. Theory Comput. 18, 3512 (2022).
[2] W. Yu, M. Govoni, J. Chem. Theory Comput. 18, 4690 (2022).
[3] B. Huang, M. Govoni, G. Galli, PRX Quantum 3, 010339 (2022).
[4] B. Huang, N. Sheng, M. Govoni, G. Galli, J. Chem. Theory Comput. 19, 1487 (2023).

Abstract category

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