First principles studies of quantum point defects

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The robust description of excited states for complex heterogeneous systems is the cornerstone of a computational framework that enables the modelling of materials for sustainable energy and quantum information science applications. I will present the simulation of optically activated processes, e.g., optical absorption and photoemission, in materials using a hierarchical modeling approach based on embedded Green's functions that relies on the combination of density functional theory, many-body perturbation theory, and multi-reference methods. I will focus on simulations of point defects in diamond and silicon carbide, which are of interest for the realization of quantum technologies. These examples benefit from the use of the latest developments in high-performance computing architectures, which include pre-exascale capable machines and quantum processors. I will discuss the impact of quantum error on the calculation of ground and excited state energies of spin-defects using noisy intermediate scale quantum computers.