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First-principles study of the energy and spin structure of excited states of NV^- center in diamond and its corresponding Hubbard model parameters SANGKOOK CHOI, MANISH JAIN, STEVEN G. LOUIE, University of California, Berkeley and Lawrence Berkeley National Laboratory — A negatively charged nitrogen-vacancy pair defect (NV) in diamond is one of the promising candidates to embody a qubit for quantum computation in solid states. It is an individually addressable quantum system that may be initialized, manipulated, and measured with high fidelity at room temperature due to a long coherence time of the spin in the ground states and long-life time of the excited states. The knowledge of the electronic and spin structures of the NV center in the ground as well as excited state is crucial in understanding them. Here, we evaluate the energies and spin structures of its excited states employing the first-principles GW-BSE methods. We further obtain the Hubbard model parameters for this defect system by comparing the excited-state energies from our ab-initio GW-BSE calculation with those from the model Hamiltonian. This work was supported by NSF Grant No. DMR10-1006184, the U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at LBNL's NERSC facility.

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