

Abstract Submitted
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Mechanism for optical initialization of spin in NV⁻ center in diamond¹ SANGKOOK CHOI, MANISH JAIN, STEVEN G. LOUIE, University of California, Berkeley and Lawrence Berkeley National Laboratory — Optical initialization of the negatively charged nitrogen-vacancy (NV⁻) center in diamond, the experimental manipulation of its degenerate mixed ground state into an un-entangled spin state through optical means, makes it one of the best candidates for realization of individually addressable spins in the solid state for quantum computing and other studies under ambient conditions. However, its exact mechanism is still not clear. Based on exact diagonalization of a many-electron Hamiltonian with parameters derived from ab initio GW calculations, the present study elucidates the electronic structure of the NV⁻ center and puts forward a concrete optical initialization mechanism. We calculated the ordering and energy surfaces of the low-energy many-body states and the relaxation processes of photo-excitation responsible for the optical initialization. Intersystem crossings are shown to be essential.

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