

Abstract Submitted
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Dynamic Jahn-Teller Effect in Negatively Charged Nitrogen-Vacancy Center in Diamond¹ TESHAYE ABTEW, PEIHONG ZHANG — The negatively charged nitrogen-vacancy (NV) center in diamond has attracted much research interest recently owing to its desirable optical properties and long spin coherent lifetime. The ground state of NV⁻ center has a ³A₂ symmetry, which can be optically excited, to a ³E state. The excited state is orbitally degenerate therefore should experience either static or dynamic Jahn-Teller (JT) effects. We use accurate first-principles methods to study structural and electronic properties of the NV⁻ center in diamond both in the ground and excited states. Our results indicate that the excited state of the NV⁻ center is indeed a dynamic JT system.

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