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First-principles anharmonic calculations and the dynamic Jahn-Teller effect JOSEPH PRENTICE, University of Cambridge, BARTOMEU MONSERRAT, Rutgers University, RICHARD NEEDS, University of Cambridge — First-principles density functional theory methods can be used to investigate the structural configurations, energetics and vibrational motions of solids, including anharmonicity, by using a vibrational self-consistent field (VSCF) method. The possibility of calculating an anharmonic vibrational wavefunction using this method allows anharmonic effects such as the dynamic Jahn-Teller effect to be described accurately. In this work, we apply our VSCF method to an important example of a dynamic Jahn-Teller system, the neutral vacancy in diamond. Our calculations demonstrate that the dynamic Jahn-Teller distorted tetrahedral structure of the vacancy is more stable than the static Jahn-Teller distorted tetragonal structure, in agreement with experimental observations, across a wide range of temperatures. This work opens the way for first-principles treatments of dynamic Jahn-Teller systems in condensed matter. Further examples of systems our method can be applied to are considered as well.

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