Erratum: *Ab initio* supercell calculations on nitrogen-vacancy center in diamond: Electronic structure and hyperfine tensors [Phys. Rev. B 77, 155206 (2008)]

Adam Gali, Maria Fyta, and Efthimios Kaxiras
(Received 19 November 2008; published 11 December 2008)

DOI: 10.1103/PhysRevB.78.239902 PACS number(s): 71.15.Mb, 99.10.Cd

In the Introduction of our paper we labeled the dangling bonds of the carbon and nitrogen atoms as σ_{1-4}, see Fig. 1. Then, we constructed an orthonormal set of states from these orbitals in Eq. (1), which we called ϕ_{1-4}. These orthonormal states are the solution of the Schrödinger equation, therefore, all the multideterminant states and their corresponding energies should be expressed in terms of ϕ_{1-4} instead of σ_{1-4}, as was accidentally done in the original paper. Therefore, in all cases that involve multideterminant states and energies, σ_{1-4} should be replaced by ϕ_{1-4}. This includes: the caption of Table I; Eqs. (2a), (2b), and (3); all four-state expressions on page 7; Eqs. (5a)–(5c) and (6).

Finally, there is a minor typographical error in the energy sequence scheme on page 7; the correct sequence is

$$\mathcal{E}[^3A_2] \xrightarrow{\approx 0.0\ \text{eV}} \mathcal{E}[^1A_1] \xrightarrow{\approx 0.9\ \text{eV}} \mathcal{E}[^1E] \xrightarrow{\approx 0.8\ \text{eV}} \mathcal{E}[^3E] \xrightarrow{\approx 0.5\ \text{eV}} \mathcal{E}'[^1E] \xrightarrow{\approx 1.3\ \text{eV}} \mathcal{E}[^1A_1].$$

These changes do not affect the conclusions of the paper.

 ©2008 The American Physical Society