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Computational Quantum Mechanics Study of Oxygen as Substitutional Atom in Diamond

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Abstract : Relatively few chemical species can be incorporated into diamond during CVD growth, and until recently the uptake of oxygen was thought to be low perhaps as a consequence of a short surface residence time. Within the literature, there is speculation regarding spectroscopic evidence for O in diamond, but no direct evidence. For example, the N3 and OK1 EPR centres have been tentatively assigned models made up from complexes of substitutional N and substitutional oxygen. In this study, we report density-functional calculations regarding the stability, electronic structures, geometry and hyperfine interaction of substitutional oxygen in diamond and show that the C2v, S=1 configuration very slightly lower in energy than the other configurations (C3v, Td, and C2v with S=0). The electronic structure of O in diamond generally gives rise to two defect-related energy states in the band gap one a non-degenerate a1 state lying near the middle of the energy gap and the other a threefold-degenerate t2 state located close to the conduction band edges. The anti-bonding a1 and t2 states will be occupied by one to three electrons for O+, O and O− respectively.

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